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INCOMPRESSIBLE SPECTRAL-ELEMENT METHOD—DERIVATION OF EQUATIONS

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ABSTRACT

A fractional-step splitting scheme breaks the full Navier-Stokes equations into explicit and implicit portions amenable to the calculus of variations. Beginning with the functional forms of the Poisson and Helmholtz equations, we substitute finite expansion series for the dependent variables and derive the matrix equations for the unknown expansion coefficients. This method employs a new splitting scheme which differs from conventional three-step (non-linear, pressure, viscous) schemes. The non-linear step appears in the conventional, explicit manner, the difference occurs in the pressure step. Instead of solving for the pressure gradient using the non-linear velocity, we add the viscous portion of the Navier-Stokes equation from the previous time step to the velocity before solving for the pressure gradient. By combining this "predicted" pressure gradient with the non-linear velocity in an explicit term, and the Crank-Nicholson method for the viscous terms, we develop a Helmholtz equation for the final velocity.

LIST OF SYMBOLS

- a = value of non-homogeneous essential boundary condition
- g = value of non-homogeneous natural boundary condition
- A = cross-sectional area
- dA = differential surface area vector
- $B_0 = 23/12$, coefficient used in Adams-Bashforth method

$B_1 = -16/12$, coefficient used in Adams-Bashforth method

$B_2 = 5/12$, coefficient used in Adams-Bashforth method

B_{abc}^{fbc} = coefficients

$(C_{ij})_{abc}^e$ = coefficients

D_n = Legendre collocation derivative of order n

D_{ij} = derivative of expansion polynomial j evaluated at node i

e_x, e_y, e_z = unit vectors in the direction of the co-ordinate axes

f = body force vector

E = total number of elements

M = moment vector

$F = -\lambda^2 \tilde{V}^{n+1}$, also represents a force vector

$J[P]$ = a functional depending on P

L = periodic length of domain

L^2 = square-integrable function

$L_k(x)$ = Legendre polynomial

i_t, j_t, k_t = the maximum number of nodes in the r, s, t directions respectively

I_n = a system of interpolating polynomials of order n

I^p_e = surface integral for side number p and element number e

\tilde{S}^e = total surface integral for element number e

$[J]$ = Jacobian matrix for the transformation between co-ordinate systems

n = surface unit normal vector

s = surface unit tangent vector

R = position vector

p = pressure

$p_i(x)$ = infinite sequence of orthogonal functions

$p(x)$, $q(x)$, $w(x)$ = functions in Sturm-Liouville equation

$P = p/\rho + \frac{1}{2}V \cdot V$, dynamic pressure

P_n = a system of orthogonal polynomials of degree n

S = an infinite system of orthogonal polynomials

t = time

Δt = time-step size

$t(n)$ = force per unit area on a surface with unit normal n

\hat{u}_i = discrete expansion coefficient for the infinite series

\bar{u}_i = discrete expansion coefficient for the finite series

V = velocity vector

\hat{V} = velocity after the non-linear step

\tilde{V} = velocity after the explicit viscous step

\check{V} = velocity after the pressure step

\bar{V} = corrected velocity after the explicit viscous step

\bar{V}_{out} = average outflow velocity correction

$U, V, W = x, y, z$ velocities respectively

w_i = weight function, integral of the expansion polynomial over domain

x, y, z = coordinates in global or physical space

x_r = partial derivative of the global co-ordinate x with respect to the local co-ordinate r

r, s, t = coordinates in local or transformed space

r_x = partial derivative of the local co-ordinate r with respect to the global co-ordinate x

Greek and other Symbols

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α = constant in homogeneous boundary condition

β = constant in homogeneous boundary condition

γ = coefficient in expansion polynomial relationships

δ = differential of a quantity

δ_{ij} = Kronecker delta

$\psi_i(x)$ = a combination of Legendre polynomials

ϵ = infinitesimal quantity

ϵ_{ijk} = alternating tensor

Ω = domain under consideration

$\partial\Omega$ = boundary of domain under consideration

$\bar{\Omega} = \Omega \cup \partial\Omega$

$\phi = V^{n+1}$

$\lambda^2 = 2/(\nu\Delta t)$

λ = eigenvalue in Sturm-Liouville equation

Λ = matrix of coefficients representing A in the expression $Ax=b$

Π = matrix of coefficients representing b in the expression $Ax=b$

ρ = fluid density

$\underline{\sigma}$ = stress tensor

σ = element surface area

$\sigma_{ij} = i, j$ component of the stress tensor

χ = moment arm

V = element volume

μ = fluid viscosity

ν = fluid kinematic viscosity

$\zeta = \zeta_x e_x + \zeta_y e_y + \zeta_z e_z$, vorticity vector

Subscripts

$_0$ = initial value

$_{\infty}$ = free-stream value

$_e$ = element number

$_n$ = direction normal to the surface

$_s$ = direction tangential to the surface

$_{ijk}$ = co-ordinate system indices

$_{in}$ = value at inlet

$_{out}$ = value at outlet

$_{wall}$ = value at wall

$_{x,y,z}$ = streamwise, vertical, and spanwise values respectively, may also refer to partial derivatives with respect to the global co-ordinates x, y, z

Superscripts

$_n$ = time step number

$_e$ = element number

$_{1,2,3,4,5,6}$ = element side numbers

INTRODUCTION

The new splitting scheme, developed by Wessel (1992), contains variations on the original three-step splitting method proposed by Korczak and Patera (1986). In the previous scheme, the non-linear, pressure, and viscous terms in the incompressible Navier-Stokes equations appear in separate fractional steps. By introducing intermediate velocities, solutions of these equations yield, consecutively, a velocity field based on the non-linear, the pressure and non-linear, and the viscous, pressure, and non-linear terms. The final step producing the true velocity field.

The velocity field resulting from the non-linear step satisfies no boundary conditions nor the incompressibility constraint. This velocity field supplies the forcing function for the Poisson equation for pressure after applying the divergence operator to the pressure step. The intermediate velocity contained in the pressure step must satisfy the divergence free constraint, thus it vanishes from the Poisson equation for pressure. Instead of solving a second-order Poisson equation for pressure, a first-order equation for pressure gradient is solved using methods from the calculus of variations—the velocity field follows directly from the pressure step. Inviscid boundary conditions on velocity determine the pressure boundary conditions; hence, errors of $O(\Delta t)$ occur near solid boundaries. Finally, the viscous step employs a Crank-Nicholson scheme yielding a Helmholtz equation with a forcing function determined by the velocity after the pressure step. Once again a variational form of the governing second-order differential equation reduces the order by one. The velocity must satisfy the full, viscous boundary conditions; however, it does not satisfy the incompressibility constraint.

The new method varies slightly from the old. Instead of solving for the pressure gradient using the non-linear velocity, we include the viscous term from the previous time step. Thus, the forcing function appearing in the Poisson equation for pressure contains contributions from both non-linear and viscous terms. The resulting pressure gradient is not solved for the velocity after the pressure step; instead, it, along with the velocity from the non-linear step, and a Crank-Nicholson method for the viscous terms, produce a Helmholtz equation for the full velocity. The boundary conditions and solution procedure remain identical to the original method. The boon comes from including the viscous

terms in the pressure gradient prediction, resulting in a quicker solution of the pressure step.

CHAPTER I

SPECTRAL APPROXIMATION

1.1 Spectral Theory

The expansion of a function u in terms of an infinite sequence of orthogonal functions $\{p_i\}$, $u = \sum_{i=-\infty}^{\infty} \hat{u}_i p_i$, underlies many numerical methods of approximation. The most familiar approximation results apply to periodic functions expanded in Fourier series. In this case, the i -th coefficient of the expansion decays faster than any inverse power of i for smooth functions with periodic derivatives. The rapid decay of the coefficients implies that the Fourier series truncated after a few terms represents a good approximation to the function. This characteristic refers to the "spectral accuracy" of the *Fourier method*.

Spectral accuracy for smooth but non-periodic functions occurs with the proper choice of expansion functions. Not all orthogonal expansion functions provide high accuracy; however, the eigenfunctions of a singular Sturm-Liouville operator allow spectral accuracy in the expansion of any smooth function, with no a priori restriction on the boundary behavior.

The expansion in terms of an orthogonal system introduces a linear transformation between u and the sequence of its expansion coefficients $\{\hat{u}_i\}$, called the *finite transform* of u between physical space and spectral space. Since the expansion coefficients depend on all the values of u in physical space, they rarely get computed exactly; instead, a finite number of approximate expansion coefficients result from using the values of u at a finite number of selected points—the nodes. This procedure defines a discrete transform between the set of values of u at the nodes and the set of approximate, or discrete coefficients.

With a proper choice of nodes and expansion functions, the finite series defined by the discrete transform represents the interpolation of u at the nodes. Maintaining spectral accuracy when replacing the finite transform with the discrete transform allows use of the interpolation series instead of the truncated series in approximating functions.

1.2 Sturm-Liouville Problems

The importance of Sturm-Liouville problems for spectral methods lies in the fact that the spectral approximation of the solution of a differential problem often occurs as a finite expansion of eigenfunctions of a suitable Sturm-Liouville problem. The general form of the Sturm-Liouville problem satisfies

$$-\frac{d}{dx}\left(p\frac{du}{dx}\right) + qu = \lambda wu \text{ in } \Omega \in (-1,1). \quad (1.2.1)$$

The real-valued functions, $p(x)$, $q(x)$, and $w(x)$, must behave properly: $p(x)$ must be continuously differentiable, strictly positive in $(-1,1)$ and continuous at $x=\pm 1$; $q(x)$ must be continuous, non-negative and bounded in $(-1,1)$; the weight function $w(x)$ must be continuous, non-negative and integrable over $(-1,1)$. The Sturm-Liouville problems of interest in spectral methods allow the expansion of an infinitely smooth function in terms of their eigenfunctions while guaranteeing spectral accuracy.

1.3 Orthogonal Systems of Polynomials

Consider the expansion of a function in terms of a system of orthogonal polynomials of degree less than or equal to n , denoted by P_n . Assume $\{p_k\}_{k=0,1,\dots}$ represents a system of algebraic polynomials (with degree of $p_k=k$) mutually orthogonal over the interval $(-1,1)$ with respect to a weight function $w(x)$. The orthogonality condition requires

$$\int_{-1}^1 p_k(x)p_m(x)w(x)dx = 0 \quad \text{whenever } m \neq k. \quad (1.3.2)$$

The formal series of a square-integrable function, $u \in L^2(-1,1)^\dagger$, in terms of the system $\{p_k\}$ appears as

$$Su = \sum_{k=0}^{\infty} \hat{u}_k p_k(x), \quad (1.3.3)$$

when the expansion coefficients \hat{u}_k satisfy

$$\hat{u}_k = \frac{1}{\|p_k\|^2} \int_{-1}^1 u(x) p_k(x) w(x) dx. \quad (1.3.4)$$

For an integer $n > 0$, the truncated series of u of order n appears as

$$P_n u = \sum_{k=0}^n \hat{u}_k p_k(x). \quad (1.3.5)$$

1.4 Gauss-Lobatto Quadratures and Discrete Polynomial Transforms

Expanding any $u(x) \in L^2(-1,1)$ in terms of the coefficients \hat{u}_k , called the *continuous expansion*, depends on the known function $u(x)$. With $u(x)$ is not known a priori, a discrete expansion for $u(x)$ —which depends on the values at the nodes—must suffice.

A close relation exists between orthogonal polynomials and Gauss-Lobatto integration formulas on the interval $[-1,1]$. Let x_0, \dots, x_n equal the roots of the $(n+1)$ -th orthogonal polynomial p_{n+1} and let w_0, \dots, w_n equal the solution of the linear system given by

$$\sum_{j=0}^n (x_j)^k w_j = \int_{-1}^1 x^k w(x) dx \quad 0 \leq k \leq n, \quad (1.4.1)$$

where $w(x)$ equals the weight function associated with the Sturm-Liouville problem, $w_j > 0$ for $j = 0, \dots, n$, and

$$\sum_{j=0}^n p(x_j) w_j = \int_{-1}^1 p(x) w(x) dx, \quad (1.4.2)$$

hold for all $p \in P_{2n+1}$. The positive numbers w_j are called "weights" (see Canuto et. al.(1988) for proof). This version of Gauss integration produces roots,

† Identifying the function $u(x)$ as "square integrable" on the given domain requires $\int_{-1}^1 |u(x)|^2 dx < \infty$.

corresponding to the collocation points, which appear in the interior of $(-1,1)$. Since boundary conditions require one or both end points, a generalized Gauss integration formula must include these points.

The Gauss-Lobatto formula considers

$$q(x) = p_{n+1}(x) + ap_n(x) + bp_{n-1}(x), \quad (1.4.3)$$

with a and b chosen so that $q(-1)=q(1)=0$. For a given weight function $w(x)$ and corresponding sequence of orthogonal polynomials p_k , $k=0, 1, 2, \dots$ we denote by x_0, \dots, x_n the nodes of the $n+1$ point integration formula of Gauss-Lobatto type, and by w_0, \dots, w_n the corresponding weights.

In a collocation method the fundamental representation of a smooth function u on $(-1,1)$ appear in terms of its values at the discrete Gauss-Lobatto points. Approximate derivatives of the function occur by analytic derivatives of the interpolating polynomial. The interpolating polynomial, denoted by $I_n u$, belongs in the set P_n and satisfies

$$I_n u(x_j) = u(x_j) \quad 0 \leq j \leq n. \quad (1.4.4)$$

Since (1.4.4) represents a polynomial of degree n , it admits an expression given by

$$I_n u = \sum_{k=0}^n \bar{u}_k p_k(x). \quad (1.4.5)$$

Since the interpolating polynomial must satisfy the function exactly at the nodes, we get

$$u(x_j) = \sum_{k=0}^n \bar{u}_k p_k(x_j), \quad (1.4.6)$$

where \bar{u}_k equal the *discrete polynomial or expansion coefficients* of u . The inverse relationship satisfies

$$\bar{u}_k = \frac{1}{\gamma_k} \sum_{j=0}^n u(x_j) p_k(x_j) w_j, \quad (1.4.7)$$

where the coefficients γ_k equal

$$\gamma_k = \sum_{j=0}^n p_k^2(x_j) w_j. \quad (1.4.8)$$

Equations (1.4.6) and (1.4.7) enabling transforms between physical space $\{u(x_j)\}$ and spectral space $\{\bar{u}_k\}$ are called the *discrete polynomial transforms* associated with the weights w_0, \dots, w_n and the nodes x_0, \dots, x_n .

1.5 Legendre Polynomials

A collection of the essential features of Legendre polynomials appears below. The Legendre polynomials $\{L_k(x), k = 0, 1, \dots\}$ equal the eigenfunctions of the singular Sturm-Liouville problem given by

$$\frac{d}{dx}[(1-x^2)\frac{d}{dx}L_k(x)] + k(k+1)L_k(x) = 0, \quad (1.5.1)$$

which equals (1.1.1) with $p(x)=1-x^2$, $q(x)=0$ and $w(x)=1$. By normalizing $L_k(x)$ so that $L_k(1)=1$, the Legendre polynomials satisfy

$$L_k(x) = \frac{1}{2^k k!} \frac{d^k}{dx^k} (x^2 - 1)^k \quad (1.5.2)$$

and represent the solution to (1.5.1) with boundary conditions (1.5.5). These polynomials also satisfy the recurrence relation, expressed as

$$L_{k+1}(x) = \frac{2k+1}{k+1} x L_k(x) - \frac{k}{k+1} L_{k-1}(x), \quad (1.5.3)$$

where $L_0(x)=1$ and $L_1(x)=x$,

$$|L_k(x)| \leq 1, \quad -1 \leq x \leq 1, \quad (1.5.4)$$

$$L_k(\pm 1) = (\pm 1)^k, \quad (1.5.5)$$

$$|L'_k(x)| \leq \frac{1}{2} k(k+1), \quad -1 \leq x \leq 1, \quad (1.5.6)$$

$$L'_k(\pm 1) = (\pm 1)^k \frac{1}{2} k(k+1), \quad (1.5.7)$$

and
$$\int_{-1}^1 L_k^2(x) dx = (k + \frac{1}{2})^{-1}, \quad (1.5.8)$$

along with the property that $L_k(x)$ is even if k is even, and odd if k is odd.

The continuous expansion of any $u \in L^2(-1,1)$ in terms of the Legendre

polynomials appears as

$$u(x) = \sum_{k=0}^{\infty} \hat{u}_k L_k(x). \quad (1.5.9)$$

Multiplying both sides by $L_j(x)$ and integrating from $x=-1$ to $x=1$, gives

$$\int_{-1}^1 u(x) L_j(x) dx = \sum_{k=0}^{\infty} \hat{u}_k \int_{-1}^1 L_j(x) L_k(x) dx, \quad (1.5.10)$$

where $w(x)=1$ according to (1.3.2). Using the orthogonal properties of the Legendre polynomials and (1.5.8) gives

$$\hat{u}_j = (j + \frac{1}{2}) \int_{-1}^1 u(x) L_j(x) dx. \quad (1.5.11)$$

The Legendre polynomials may appear directly as the expansion functions of (1.5.9) or as a combination of Legendre polynomials which satisfy

$$\psi_j(x_i) = \delta_{ij}, \quad (1.5.12)$$

where $\psi(x)$ equals

$$\psi_j(x) = \frac{1}{n(n+1)L_n(x_j)} \left(\frac{1-x^2}{x-x_j} \right) \frac{d}{dx} L_n(x). \quad (1.5.13)$$

This later form allows simpler implementation. The nodes $\{x_j\}$, $j=1, \dots, n-1$, equal the zeros of $\frac{d}{dx} L_n(x)$, with $x_0=-1$, and $x_n=1$. The quadrature weights, shown in (1.4.2), satisfy

$$\sum_{k=0}^n \psi_j(x_k) w_k = \int_{-1}^1 \psi_j(x) w(x) dx. \quad (1.5.14)$$

Since the Legendre polynomials correspond to $w(x)=1$, and the expansion polynomials satisfy the relation $\psi_j(x_k)=\delta_{kj}$, (1.5.14) reduces to

$$\sum_{k=0}^n \delta_{kj} w_k = \int_{-1}^1 \psi_j(x) dx \quad (1.5.15)$$

or

$$w_j = \int_{-1}^1 \psi_j(x) dx. \quad (1.5.16)$$

Inserting the expression for the expansion polynomial, (1.5.13), gives after integration

$$w_j = \frac{2}{n(n+1)} \frac{1}{L_n(x_j)^2}, \quad j=0, \dots, n \quad (1.5.17)$$

for the quadrature weights. The normalization factors γ_k , introduced in (1.4.8) for the general Sturm-Liouville problem, equal

$$\gamma_k = (k + \frac{1}{2})^{-1}, \quad \text{for } k < n \quad (1.5.18)$$

and $\gamma_n = 2/n. \quad (1.5.19)$

for the specific polynomials given in (1.5.13).

1.6 Differentiation Using Legendre Polynomials

Differentiation may occur in either spectral space or physical space.

Differentiation in spectral space consists of computing the Legendre expansion of the derivative of a function in terms of the Legendre expansion of the function itself. For example, if $u(x) = \sum_{k=0}^{\infty} \hat{u}_k L_k(x)$, $\frac{du}{dx}$ can be represented as

$$\sum \frac{du}{dx} = \frac{du}{dx} = \sum_{k=0}^{\infty} \frac{d}{dx} (\hat{u}_k) L_k(x), \quad (1.6.1)$$

where

$$\frac{d}{dx} \hat{u}_k = (2k+1) \sum_{p=k+1}^{\infty} \hat{u}_p, \quad p+k \text{ odd}. \quad (1.6.2)$$

The proof of (1.6.2) begins with a relation between Legendre polynomials and their derivatives:

$$(2k+1)L_k(x) = \frac{d}{dx} L_{k+1}(x) - \frac{d}{dx} L_{k-1}(x), \quad k \geq 0. \quad (1.6.3)$$

Substituting this expression for $L_k(x)$ into (1.6.1) gives

$$\begin{aligned} \frac{d}{dx} u(x) &= \sum_{k=0}^{\infty} \frac{d\hat{u}_k}{dx} \frac{1}{2k+1} \frac{d}{dx} L_{k+1}(x) \\ &\quad - \sum_{k=0}^{\infty} \frac{d\hat{u}_k}{dx} \frac{1}{2k+1} \frac{d}{dx} L_{k-1}(x) \end{aligned} \quad (1.6.4)$$

which upon changing the limits of the summation gives

$$\begin{aligned} \frac{d}{dx} u(x) &= \sum_{k=1}^{\infty} \frac{d\hat{u}_{k-1}}{dx} \frac{1}{2k-1} \frac{d}{dx} L_k(x) \\ &\quad - \sum_{k=-1}^{\infty} \frac{d\hat{u}_{k+1}}{dx} \frac{1}{2k+3} \frac{d}{dx} L_k(x). \end{aligned} \quad (1.6.5)$$

Combining both terms gives

$$\frac{d}{dx}u(x) = \sum_{k=1}^{\infty} \left[\frac{d\hat{u}_{k-1}/dx}{2k-1} - \frac{d\hat{u}_{k+1}/dx}{2k+3} \right] \frac{d}{dx}L_k(x) \quad (1.6.6)$$

where both the terms corresponding to $k=0$ and -1 vanishes since $\frac{d}{dx}L_0(x)=0$ and $\frac{d}{dx}L_{-1}(x)=0$.[†] This expression represents the derivative of $u(x)$ in spectral space.

In physical space, the derivative appears as

$$\frac{d}{dx}(Su) = \frac{d}{dx}u(x) = \sum_{k=0}^{\infty} \hat{u}_k \frac{d}{dx}L_k(x). \quad (1.6.7)$$

Equating (1.6.6) and (1.6.7), and recognizing that $\frac{d}{dx}L_0(x)=0$, gives

$$\sum_{k=1}^{\infty} \hat{u}_k \frac{d}{dx}L_k(x) = \sum_{k=1}^{\infty} \left[\frac{d\hat{u}_{k-1}/dx}{2k-1} - \frac{d\hat{u}_{k+1}/dx}{2k+3} \right] \frac{d}{dx}L_k(x). \quad (1.6.8)$$

Since the $L_k(x)$ equal the eigenfunctions of Sturm-Liouville problem, they, along with their derivatives, form a linearly independent or orthogonal set. Therefore, multiplying (1.6.8) by $\frac{d}{dx}L_j(x)$ and integrating from -1 to 1 results in

$$\hat{u}_k = \frac{d\hat{u}_{k-1}/dx}{2k-1} - \frac{d\hat{u}_{k+1}/dx}{2k+3}. \quad (1.6.9)$$

Evaluating (1.6.2) with $n=k+1$ gives

$$\frac{d}{dx}\hat{u}_{n-1} = (2n-1) \sum_{p=n}^{\infty} \hat{u}_p, \quad p+n \text{ even}; \quad (1.6.10)$$

similarly, (1.6.2) evaluated using $n=k-1$ yields

$$\frac{d}{dx}\hat{u}_{n+1} = (2n+3) \sum_{p=n+2}^{\infty} \hat{u}_p, \quad p+n \text{ even}. \quad (1.6.11)$$

Substituting (1.6.10) and (1.6.11) into (1.6.9) gives

$$\hat{u}_n = \sum_{p=n}^{\infty} \hat{u}_p - \sum_{p=n+2}^{\infty} \hat{u}_p, \quad p+n \text{ even}, \quad (1.6.12)$$

which reduces to $\hat{u}_n = \hat{u}_n$. This completes the proof of (1.6.2). The two derivative expressions given by (1.6.1) and (1.6.7) produce different results in practice:

[†]For $k=-1$ we have $dL_{-1}(x)/dx = c/(1-x^2)$, where c equals a constant. Since the boundary conditions are $dL_k(\pm 1)/dx = (\pm 1)^k k(k+1)/2$ which equals zero for $k=-1$, we see that the constant c must equal zero.

$$\frac{d}{dx}(P_n u) \neq P_n \frac{du}{dx}. \quad (1.6.13)$$

The quantity on the left equals the *Legendre Galerkin* derivative. The error, $\frac{d}{dx}(P_n u) - P_n \frac{du}{dx}$ decays spectrally for infinitely smooth solutions. However, for functions, u , with finite regularity (not infinitely periodic) this difference decays at a slower rate than the truncation error for the derivative $\frac{du}{dx} - P_n \frac{du}{dx}$. Thus $\frac{d}{dx}(P_n u)$ is asymptotically a worse approximation to $\frac{du}{dx}$ than $P_n \frac{du}{dx}$ (see Canuto et. al. (1988)).

1.7 Legendre Derivatives at the Nodes

Approximate differentiation in physical space occur by differentiating the interpolation $I_n u$ (as defined in (1.4.5)) and evaluating it at the nodes. This resulting polynomial of degree $n-1$, represented as

$$D_n u = \frac{d}{dx}(I_n u), \quad (1.7.1)$$

and called the *Legendre collocation* derivative of u relative to the chosen set of nodes, differs from the *Galerkin* derivative $\frac{d}{dx}(P_n u)$ since the latter depends on the continuous coefficients \hat{u}_k and the former on the discrete coefficients \bar{u}_k .

One method for obtaining the collocation derivative, involves computing the values $(D_n u)(x_i)$, ($i = 0, \dots, n$) from the values $u(x_j)$, ($j = 0, \dots, n$), by employing (1.4.7) for the discrete Legendre coefficients \bar{u}_j , and (1.6.2) for the discrete derivative coefficients $\frac{d}{dx}\bar{u}_j$, and computing $(D_n u)_i$ from

$$(D_n u)(x_i) = \sum_{k=0}^n \frac{d}{dx}(\bar{u}_k) \psi_k(x_i). \quad (1.7.2)$$

A preferred option involves the collocation derivative at the nodes through matrix multiplication. It appears as

$$(D_n u)(x_i) = \sum_{k=0}^n \bar{u}_k \frac{d}{dx}[\psi_k(x)]|_{x=x_i} \quad (1.7.3)$$

for $i=0, \dots, n$. When $D_{ik} = \frac{d}{dx}\psi_k(x_i)$, (1.7.3) equals

$$(D_n u)(x_i) = \sum_{k=0}^n \tilde{u}_k D_{ik}, \text{ for } i = 0, \dots, n. \quad (1.7.4)$$

Using (1.5.13) for $\psi_k(x)$ gives

$$D_{ik} = \begin{cases} \frac{L_n(x_i)}{L_n(x_k)} \frac{1}{x_i - x_k}, & i \neq k. \\ \frac{(n+1)n}{4}, & i = k = 0. \\ -\frac{(n+1)n}{4}, & i = k = n. \\ 0, & \text{otherwise.} \end{cases} \quad (1.7.5)$$

1.8 Integration Using Legendre Polynomials

Integration in transform space consists of computing the integral of the Legendre expansion of a function. If $u(x) \approx \sum_{k=0}^n \tilde{u}_k \psi_k(x)$, the integral over the domain $x \in [-1, 1]$ equals

$$\int_{-1}^1 u(x) dx \approx \int_{-1}^1 \sum_{k=0}^n \tilde{u}_k \psi_k(x) dx. \quad (1.8.1)$$

Assuming the series converges, integration and summation may change places, giving

$$\int_{-1}^1 u(x) dx \approx \sum_{k=0}^n \tilde{u}_k \int_{-1}^1 \psi_k(x) dx. \quad (1.8.2)$$

Using the integral of the expansion function according to (1.5.16) gives

$$\int_{-1}^1 u(x) dx \approx \sum_{k=0}^n \tilde{u}_k w_k. \quad (1.8.3)$$

CHAPTER II

SPECTRAL ELEMENT METHOD

2.1 Introduction

The spectral-element method, a variational procedure in which the approximating functions depend on representing the given domain as a collection of simple sub-domains, differs from both spectral methods and finite-element methods in two ways: (1) pure spectral methods employ high degree approximating functions with support defined over the entire domain, and (2) finite-element methods use low degree approximating functions with compact support (i.e., a given element's approximating functions differ from zero only within the element). Spectral-element methods exploit the advantage of high degree functions inherent in pure spectral methods, along with the flexibility finite-element methods provide in representing complex domains. The sub-domains, or finite elements, equal geometrically simple shapes that permit a systematic construction of the approximating functions. These ecumenical functions satisfy all boundary conditions and problem data by employing concepts of orthogonal polynomials from Sturm-Liouville theory. On an elemental basis, the dependent variables appear as a finite sequence of the approximation functions with coefficients representing the dependent variables at a finite number of preselected points (i.e., nodes, whose number and location dictates the degree and form of the approximating functions).

2.2 Partitioning of Domain

One feature of the spectral-element method distinguishing it from the pure spectral method allows representing the given domain by a collection of sub-domains. A subsequent transformation maps each sub-domain from the physical

(x,y,z) space to the local (r,s,t) space by an isoparametric mapping. The subdomains in local space equal simple geometries, such as cubes in three-dimensional space. Two important features in typical geometries dictate this mapping: first, the definition of the approximation functions from Sturm-Liouville equations only apply to certain well-defined geometries; and second, an arbitrary domain cannot accept a collection of simple domains without introducing error. By defining the approximating functions element-wise, the accuracy of the approximation improves by increasing either the number of elements (i.e., refining the mesh) or the degree of the approximating functions.

In mathematical terms, the total domain $\bar{\Omega} = \Omega \cup \partial\Omega$ splits into a finite number, E , of subsets, $\bar{\Omega}_e$, called finite elements, such that: each $\bar{\Omega}_e$ is closed and non-empty; the boundary $\partial\Omega_e$ of each $\bar{\Omega}_e$ is Lipschitz-continuous (no singularities, cusps, et cetera); the intersection of any two distinct elements is empty, i.e., $\Omega_e \cap \Omega_f = \emptyset$, $e \neq f$; and the union $\bar{\Omega}$ of all elements $\bar{\Omega}_e$ equals the total domain, given as

$$\bar{\Omega} = \sum_{e=1}^E \bar{\Omega}_e. \quad (2.2.1)$$

We could not satisfy the last property without the mapping between physical and local space.

2.3 Spectral-Element Interpolation

By allowing the possibility that each element represents the entire domain with the general boundary conditions of the differential equation, the essential boundary conditions equal the values of the independent variables at the nodes, while the natural boundary conditions get subsumed into the variational form of the equation over the element. After assembling the elements, the boundary values on portions of the boundaries of elements sharing the boundary of the

given domain are replaced by the actual specified values (imposition of boundary conditions).

In the spectral-element method, the minimum degree of the algebraic approximating functions depends on the order of the differential equation being solved, and the degree of the polynomial in turn dictates the number of interpolation points, called nodes, to be identified in the element.

The approximation functions, also called interpolation functions, depend on interpolation of the function and possibly its derivatives at the nodes of the element. The nodes placed along the boundary of the element uniquely define the element geometry. Place any additional nodes required to define the interpolation functions at other points, either in the interior or on the boundary. The boundary nodes also enable the connection of adjacent elements by requiring equality of the primary degrees of freedom (i.e., variables that appear in essential boundary condition) at nodes shared by any two elements. Thus, we cannot accurately represent discontinuous primary variables. Such problems arise in, for example, the study of compressible flow where shock waves contain velocity discontinuities. These functions make poor primary variables in the spectral-element model unless we employ special procedures during assembly.

For each Ω_e , let P_n^e denote the finite-dimensional spaces spanned by linearly independent local interpolation functions $\{\psi_i^e\}_{i=0}^n$ of the nodal points. Over each element $\bar{\Omega}_e \subset \bar{\Omega}$ the approximation $I_n u^e$ of u^e equals

$$u^e \approx I_n u^e = \sum_{i=0}^n \bar{u}_i^e \psi_i^e(r), \quad (2.3.1)$$

where the local expansion coefficients \bar{u}_i^e equal the values of u^e at the preselected nodes $\{r_i^e\}$ in the element $\bar{\Omega}_e$. As indicated in §1.5, the interpolation functions satisfy

$$\psi_i^e(r_j) = \delta_{ij}, \quad (2.3.2)$$

where δ_{ij} is the Kronecker-delta function.

2.4 Connectivity (or Assembly) of Elements

As mentioned earlier, all elements contain boundary nodes defining their geometry and allowing connection with their neighbors. The connectivity of elements requires equal values of the primary variables in nodes common to adjacent elements. Assembling the unique sub-domains into the entire domain, a process known as *direct stiffness*, requires the identification of a universal or global system of nodes, and a corresponding set of global expansion coefficients for the primary variables. The resulting matrix expression relates the global expansion coefficients to the parameters of the governing differential equation and boundary conditions.

As indicated earlier, the primary variables, those associated with the essential boundary conditions, appear as the global expansion coefficients of the assembled matrix relation. The secondary variables appear in the natural boundary conditions.

2.5 Isoparametric Formulation

Isoparametric schemes use the same interpolation functions to represent both the co-ordinate mapping and the primary variables. Thus, the physical space x maps into the local r co-ordinate system by

$$x^e \approx I_n x^e = \sum_{i=0}^n \bar{x}_i^e \psi_i^e(r), \quad (2.5.1)$$

when primary variables appear as

$$u^e \approx I_n u^e = \sum_{i=0}^n \bar{u}_i^e \psi_i^e(r). \quad (2.5.2)$$

CHAPTER III

TIME-SPLITTING SCHEME FOR THE NAVIER-STOKES EQUATIONS

3.1 Governing Equations and Boundary Conditions

According to the formulation given below, the domain under consideration, $\Omega \subset \mathbb{R}^3$ with boundary $\partial\Omega$, may translate but not deform. The Navier-Stokes equations on the closed domain, $\bar{\Omega} = \Omega \cup \partial\Omega$, consist of the constant density *continuity* equation given by

$$\nabla \cdot \mathbf{V} = 0, \quad (3.1.1)$$

and the corresponding *momentum* equation expressed as

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} = -\frac{\nabla p}{\rho} + \mathbf{f} + \nu \nabla^2 \mathbf{V}. \quad (3.1.2)$$

Introducing

$$\mathbf{V} \times \nabla \times \mathbf{V} = -(\mathbf{V} \cdot \nabla) \mathbf{V} + \frac{1}{2} \nabla (\mathbf{V} \cdot \mathbf{V}) \quad (3.1.3)$$

into the momentum equation gives

$$\frac{\partial \mathbf{V}}{\partial t} = \mathbf{V} \times \nabla \times \mathbf{V} - \nabla \left(\frac{p}{\rho} + \frac{1}{2} \mathbf{V} \cdot \mathbf{V} \right) + \mathbf{f} + \nu \nabla^2 \mathbf{V}, \quad (3.1.4)$$

in which both \mathbf{V} and p along with the body force, \mathbf{f} , depend on both position in the fluid and time.

The physical boundary conditions for a given problem must allow us to divide the entire boundary into regions associated with essential boundary conditions (e.g., walls and inlets), natural boundary conditions (e.g., outlets and free-streams), and periodicity boundary conditions. The numerical procedure handles each of these regions separately.

The essential boundary conditions appear as

$$\mathbf{V} = \mathbf{V}_{\text{wall}} \quad (3.1.5)$$

on solid wall boundaries, and

$$\mathbf{V} = \mathbf{V}_{\text{in}} \quad (3.1.6)$$

on inlet boundaries. The natural boundary condition at the outflow equals

$$(\mathbf{n} \cdot \nabla) \mathbf{V} = 0, \quad (3.1.7)$$

where \mathbf{n} is the outward surface normal vector, and along the free stream

$$\mathbf{n} \cdot \mathbf{V} = \mathbf{n} \cdot \mathbf{V}_{\text{boundary}} \quad (3.1.8)$$

and

$$\mathbf{n} \times (\underline{\sigma} \cdot \mathbf{n}) = 0, \quad (3.1.9)$$

where $\underline{\sigma}$ equals the local stress tensor. Equation (3.1.9) expresses the fact that the stress at the free stream must lie entirely normal to the boundary. By manipulating the pair of conditions (3.1.8) and (3.1.9) we can show that they equal the homogeneous natural condition on velocity, $(\mathbf{n} \cdot \nabla) \mathbf{V} = 0$, (see appendix C). The boundary condition along periodic surfaces equals

$$\mathbf{V}(\mathbf{x} + \mathbf{L}) = \mathbf{V}(\mathbf{x}), \quad (3.1.10)$$

where \mathbf{L} equals the relative position vector between the two periodic boundaries. All of these conditions refer to velocity; pressure boundary conditions depend on the governing equations. Finally, the initial conditions equal $\mathbf{V}(\mathbf{x}, t=0) = \mathbf{V}_0(\mathbf{x})$ for $\mathbf{x} \in \Omega \subset \mathbb{R}^3$.

3.2 Splitting Method

In the variational solution of time-dependent problems, we represent the dependent variables in a finite dimensional vector space. The undetermined coefficients depend on time, while the base functions depend on spatial coordinates. This leads to a two-stage approximation, both of which could employ variational methods. We choose to discretize the equations in space and iterate in time, thus giving a spatial variational problem. Such a procedure, commonly known as a *semi-discrete approximation*, results in a set of ordinary differential equations in time.

No variational form exists for the full momentum equation; therefore, we split it into simple forms and apply variational techniques to each portion individually. Employing the splitting scheme followed by Wessel (1992), we introduce intermediate velocities, \hat{V} , \tilde{V} , \check{V} , and \bar{V} , which allows splitting of the momentum equation into fractional steps. The scheme employs a "predictor-corrector" approach whereby the predicted velocity at time step $n+1$, which results from sequentially computing intermediate velocities based on the non-linear terms, the viscous terms, and the pressure terms, determines the pressure gradient. The corrected velocity depends on this predicted pressure gradient. A brief explanation follows. The first, or *non-linear*, step appears as

$$\frac{\hat{V}^{n+1} - V^n}{\Delta t} = V^n \cdot \nabla \times V^n + f^{n+1}; \quad (3.2.1)$$

the second, or *viscous*, step equals

$$\frac{\tilde{V}^{n+1} - \hat{V}^{n+1}}{\Delta t} = \nu \nabla^2 V^n; \quad (3.2.2)$$

and the third, or *pressure*, step includes

$$\frac{\check{V}^{n+1} - \tilde{V}^{n+1}}{\Delta t} = -\nabla \left(\frac{P^{n+1}}{\rho} + \frac{1}{2} V^{n+1} \cdot V^{n+1} \right) = -\nabla P^{n+1}. \quad (3.2.3)$$

The velocity after the pressure step, \check{V}^{n+1} , must satisfy the divergence-free constraint. By applying the divergence operator to (3.2.3), a relationship between pressure and \check{V}^{n+1} ensues. The solution of this Poisson equation for pressure determines the predicted pressure gradient. Using the previously computed velocity after the non-linear step and this new pressure gradient, a new velocity results after adding the explicit viscous term:

$$\frac{\bar{V}^{n+1} - \check{V}^{n+1}}{\Delta t} = -\nabla P^{n+1} + \frac{1}{2} \nu \nabla^2 V^n. \quad (3.2.4)$$

We still must add another $\frac{1}{2} \nu \nabla^2 V$ to the right-hand side to yield the full Navier-Stokes equation. We use the Crank-Nicholson method by adding $\frac{1}{2} \nu \nabla^2 V^{n+1}$ to

the velocity \tilde{V}^{n+1} giving an implicit viscous step appearing as

$$\frac{V^{n+1} - \tilde{V}^{n+1}}{\Delta t} = \frac{1}{2} \nu \nabla^2 V^{n+1}. \quad (3.2.5)$$

We benefit from this splitting scheme by representing the implicit viscous and pressure steps in time-independent, elliptic form: the viscous step in the form of Helmholtz's equation, and the pressure step as Poisson's equation. We express both equations in variational form and solve them by finding the extremum of the corresponding functional. Some of the details of each of the five steps appear below. The two steps containing the explicit viscous terms require no exposition.

3.3 Non-Linear Step

We solve the non-linear advective term explicitly using a three-step Adams-Bashforth method given by

$$\frac{\hat{V}^{n+1} - V^n}{\Delta t} = B_0(V \times \nabla \times V + f)^n + B_1(V \times \nabla \times V + f)^{n-1} + B_2(V \times \nabla \times V + f)^{n-2}. \dagger$$

This hyperbolic operator imposes stability conditions, in the form of a Courant-Friedrich-Lewy number, on the scheme. Neither boundary conditions nor continuity constraints apply to \hat{V}^{n+1} .

3.4 Pressure Step

The velocity after the pressure step, \tilde{V} , must satisfy the zero divergence constraint. Applying the divergence operator to (3.2.2) gives

$$\nabla \cdot \left(\frac{\tilde{V}^{n+1} - \hat{V}^{n+1}}{\Delta t} \right) = \nabla \cdot (-\nabla P^{n+1}). \quad (3.4.1)$$

Since \tilde{V} does not satisfy the zero divergence constraint, (3.4.1) simplifies to

$$\frac{\nabla \cdot \tilde{V}^{n+1}}{\Delta t} = \nabla \cdot \nabla P^{n+1}. \quad (3.4.2)$$

The boundary conditions on pressure depend on the governing equations.

\dagger The three-step Adams-Bashforth coefficients equal $B_0=23/12$, $B_1=-16/12$, and $B_2=5/12$.

We obtain the pressure boundary conditions by taking the inner product of (3.1.4) with the surface outward unit normal \mathbf{n} and rearranging. This yields

$$\mathbf{n} \cdot \nabla P = -\frac{\partial}{\partial t}(\mathbf{n} \cdot \mathbf{V}) + \nu \mathbf{n} \cdot \nabla^2 \mathbf{V} + \mathbf{n} \cdot \mathbf{f} + \mathbf{n} \cdot (\mathbf{V} \times \nabla \times \mathbf{V}). \quad (3.4.3)$$

This expression represents the exact physical boundary condition on pressure obtained from the governing differential equation. Unfortunately, we cannot use this form since some of the terms on the right-hand side remain unknown.

Therefore, the numerical procedure uses a simplified form which neglects the viscous term, the body force, and the non-linear term:

$$\mathbf{n} \cdot \nabla P = -\frac{\partial}{\partial t}(\mathbf{n} \cdot \mathbf{V}). \quad (3.4.4)$$

When we discretize this equation in time by writing the time derivative of velocity as $(\mathbf{V}^{n+1} - \mathbf{V}^n)/\Delta t$, we see that unknown terms still remain on the right-hand side. By further approximating the time-derivative using intermediate velocities we obtain

$$\mathbf{n} \cdot \nabla P = -\mathbf{n} \cdot (\tilde{\mathbf{V}}^{n+1} - \tilde{\mathbf{V}}^n)/\Delta t. \quad (3.4.5)$$

It appears that we still do not know $\tilde{\mathbf{V}}^{n+1}$ at this point; however, a careful vetting of the various boundary conditions reveals otherwise. This mathematical approximation to the physical boundary condition may be good or bad depending on the characteristics of the flow as indicated below. Where essential boundary conditions occur $\mathbf{n} \cdot \tilde{\mathbf{V}}^{n+1}$ equals $\mathbf{n} \cdot \mathbf{V}_{\text{wall}}$ or $\mathbf{n} \cdot \mathbf{V}_{\text{inlet}}$, and (3.4.5) becomes

$$\mathbf{n} \cdot \nabla P = -\mathbf{n} \cdot (\mathbf{V}_{\text{wall}} - \tilde{\mathbf{V}}^n)/\Delta t. \quad (3.4.6)$$

This term differs from the true physical boundary condition at a solid surface (or at the inlet if $\mathbf{n} \cdot (\mathbf{V} \times \nabla \times \mathbf{V}) = 0$) since it lacks both the viscous term, $\nu \mathbf{n} \cdot \nabla^2 \mathbf{V}$, and the body-force term, $\mathbf{n} \cdot \mathbf{f}$. For a flow with no body force, the approximate boundary condition differs from the physical boundary condition by the viscous term. In other words, the mathematical boundary condition equals the inviscid

boundary condition along solid walls. Deville and Orszag (1980) showed that this approximation introduces a time-splitting error $O(1)$ in $\mathbf{n} \cdot \nabla^2 \mathbf{V}$ over a layer of thickness $O(\sqrt{\Delta t \nu})$. No error estimate exists at the outlet since even the physical boundary conditions remain unknown.

Along the free-stream the viscous term remains negligibly small under most circumstances;‡ while the advection term, $\mathbf{n} \cdot (\mathbf{V} \times \nabla \times \mathbf{V})$, equals zero, since \mathbf{n} and $\mathbf{V} \times \nabla \times \mathbf{V}$ are perpendicular.‡‡ Furthermore, when the body force is perpendicular to the free-stream boundary—as in most flows—the body-force term vanishes, and the simplified boundary condition equals the physical one.

Along exit boundaries where natural conditions get specified, the terms neglected by the approximate pressure boundary condition do not vanish. However, their influence remains confined to a region near the boundary, since convection sweeps any induced errors out of the domain.

3.5 Viscous Step

The implicit viscous step appears as

‡The viscous term equals $\mathbf{n} \cdot \nabla^2 \mathbf{V}$. The velocity can be written in terms of a local co-ordinate system where \mathbf{n} equals the normal to the surface and \mathbf{s} lies tangential to the surface. Hence $\mathbf{V} = V_s \mathbf{s} + V_n \mathbf{n}$, and $\mathbf{n} \cdot \nabla^2 \mathbf{V} = \mathbf{n} \cdot [(\partial^2 V_s / \partial s^2 + \partial^2 V_s / \partial n^2) \mathbf{s} + (\partial^2 V_n / \partial s^2 + \partial^2 V_n / \partial n^2) \mathbf{n}]$. The first term is zero because \mathbf{s} and \mathbf{n} remain perpendicular. The second term vanishes in most common flows. For example, when a homogeneous body force or a body force with a vanishing or zero gradient near the free-stream boundary (e.g., the "Blasius" body force) forces the flow, the second derivatives of V_n vanish sufficiently far from disturbance generating structures. Likewise, when the free-stream boundary represents a moving plate, as in Couette flow, $\partial^2 V_n / \partial s^2$ usually equals zero, and $\partial^2 V_n / \partial n^2$ again vanishes far away from the disturbance generating structures.

‡‡The boundary conditions specified along a free stream reduce to $\mathbf{n} \cdot \nabla \mathbf{V} = 0$, according to the results of appendix C. Thus, the gradient of velocity lies parallel to the surface, or alternatively, the cross product of ∇ and \mathbf{V} lies parallel to \mathbf{n} (the zero normal velocity constraint requires \mathbf{V} to lie in the plane of the boundary). Therefore, the cross product of \mathbf{V} and $\nabla \times \mathbf{V}$ lies in the plane of the surface, or perpendicular to \mathbf{n} . Whence $\mathbf{n} \cdot (\mathbf{V} \times \nabla \times \mathbf{V}) = 0$.

$$\frac{V^{n+1} - \tilde{V}^{n+1}}{\Delta t} = \frac{1}{2}\nu \nabla^2 V^{n+1}. \quad (3.5.1)$$

This implicit equation remains unconditionally stable. Therefore, we could avoid unreasonable time step restrictions due to the high spatial resolution of spectral approximations near the boundaries of elements save the other explicit steps.

The boundary conditions on the velocity after the viscous step, V^{n+1} , equal the physical boundary conditions given in §3.1. In formulating the viscous step, we did not subsume the zero divergence condition into the expression for V^{n+1} .

Hence, V^{n+1} does not satisfy the Navier-Stokes equations exactly. Normally, this error does not dominate the solution since the velocity after the viscous step nearly equals the zero divergence velocity, \tilde{V}^{n+1} . Amon (1988) observed that the divergence of V^{n+1} remains a few orders-of-magnitude smaller than that of \tilde{V}^{n+1} . We transform (3.5.1) into Helmholtz's equation by adding $-\tilde{V}^{n+1}$ to both sides of (3.5.1) giving

$$-\tilde{V}^{n+1} = -V^{n+1} + \frac{1}{2}\nu\Delta t \nabla^2 V^{n+1}. \quad (3.5.3)$$

Rearranging yields

$$\nabla^2 \phi - \frac{2}{\nu\Delta t} \phi = -\frac{2}{\nu\Delta t} \tilde{V}^{n+1}, \quad (3.5.4)$$

which appears as

$$\nabla^2 \phi - \lambda^2 \phi = F, \quad (3.5.5)$$

when $\phi = V^{n+1}$, $\lambda^2 = \frac{2}{\nu\Delta t}$ and $F = -\lambda^2 \tilde{V}^{n+1}$. Since ϕ depends on the velocity satisfying the physical boundary conditions, the condition on ϕ associated with essential boundary conditions equals

$$\phi = V_{\text{wall}} \text{ or } V_{\text{inlet}}. \quad (3.5.6)$$

The exit, or natural, boundary condition equals

$$\mathbf{n} \cdot \nabla \phi = 0, \quad (3.5.7)$$

which also satisfies the free-stream boundary conditions when the free-stream

condition on velocity behaves according to the restrictions given in appendix C.

The periodic boundary conditions equal $\phi(\mathbf{x}+\mathbf{L})=\phi(\mathbf{x})$, where \mathbf{L} equals the relative position vector between the two boundaries.

CHAPTER IV

NON-LINEAR STEP

4.1 Introduction

The non-linear step, the only explicit part of the three-step time-splitting scheme, introduces a time-step size stability restriction. Since only first-order derivatives appear, no benefit accrues from casting the governing equation in "weak" form; instead, we apply a collocation variational approach. (When the governing equation has an equivalent "weak" form, we may multiply it by a suitably differentiable test function, integrate over the appropriate domain, and then integrate by parts. The resulting variational form contains derivatives of lower order than the original equation.) In the collocation technique, the test function equals the Dirac-delta function. Since this function has no derivative, the resulting solution must contain as many derivatives as the order of the governing differential equation. For this first-order equation, therefore, the solution occupies the space of functions $H^1(\Omega)$.

4.2 Variational Form

The Adams-Bashforth three-step procedure applied to the non-linear portion of the split Navier-Stokes equation appears in §3.3 and equals

$$\hat{V}^{n+1} - V^n = B_0 \Delta t (V \times \nabla \times V + f)^n + B_1 \Delta t (V \times \nabla \times V + f)^{n-1} + B_2 \Delta t (V \times \nabla \times V + f)^{n-2}. \quad (4.2.1)$$

To transform this equation into variational form, we multiply by a test function, $\psi \in H(\Omega)$, and integrating over the entire domain, giving

$$\int_{\Omega} [\hat{V}^{n+1} - V^n - B_0 \Delta t (V \times \nabla \times V + f)^n - B_1 \Delta t (V \times \nabla \times V + f)^{n-1} - B_2 \Delta t (V \times \nabla \times V + f)^{n-2}] \psi dV = 0. \quad (4.2.2)$$

The collocation method uses $\psi_i = \delta(\mathbf{x} - \mathbf{x}_i)$, where the \mathbf{x}_i 's equal the locations of

the nodal points where the differential equation is satisfied exactly. Introducing $\psi_i = \delta(\mathbf{x} - \mathbf{x}_i)$ into (4.2.2) and integrating results in the discrete form of the differential equation in terms of the unknown expansion coefficients \tilde{V}_{ijk} and \tilde{V}_{ijk} . Products, such as $\mathbf{V} \times \nabla \times \mathbf{V}$, also appear in terms of their coefficients at the nodes. The result equals

$$\tilde{V}_{ijk}^n - \tilde{V}_{ijk}^{n-1} = \quad (4.2.3)$$

$$B_0 \Delta t (\tilde{\mathbf{V}} \times \nabla \times \tilde{\mathbf{V}} + \mathbf{f})_{ijk}^n + B_1 \Delta t (\tilde{\mathbf{V}} \times \nabla \times \tilde{\mathbf{V}} + \mathbf{f})_{ijk}^{n-1} + B_2 \Delta t (\tilde{\mathbf{V}} \times \nabla \times \tilde{\mathbf{V}} + \mathbf{f})_{ijk}^{n-2}.$$

We explore the spatial discretization of the various quantities in the following sections.

4.3 Spatial Discretization of Vorticity

Express the vorticity, $\nabla \times \mathbf{V}$, in Cartesian co-ordinates as

$$\nabla \times \mathbf{V} = \left(\frac{\partial W}{\partial y} - \frac{\partial V}{\partial z} \right) \mathbf{e}_x + \left(\frac{\partial U}{\partial z} - \frac{\partial W}{\partial x} \right) \mathbf{e}_y + \left(\frac{\partial V}{\partial x} - \frac{\partial U}{\partial y} \right) \mathbf{e}_z, \quad (4.3.1)$$

where the partial derivatives refer to the global co-ordinate system. We must transform these derivatives from the global, or physical, co-ordinate system to the local (r,s,t) system. According to appendix A, the partial derivatives expressed in terms of the local co-ordinates equal

$$\frac{\partial^e}{\partial x} = r_x^e \frac{\partial^e}{\partial r} + s_x^e \frac{\partial^e}{\partial s} + t_x^e \frac{\partial^e}{\partial t}, \quad (4.3.2a)$$

$$\frac{\partial^e}{\partial y} = r_y^e \frac{\partial^e}{\partial r} + s_y^e \frac{\partial^e}{\partial s} + t_y^e \frac{\partial^e}{\partial t}, \quad (4.3.2b)$$

$$\text{and} \quad \frac{\partial^e}{\partial z} = r_z^e \frac{\partial^e}{\partial r} + s_z^e \frac{\partial^e}{\partial s} + t_z^e \frac{\partial^e}{\partial t}. \quad (4.3.2c)$$

(The superscript e refers to the element number.) Introducing these expressions into (4.3.1) gives

$$(4.3.3)$$

†The time step number replaces the element superscript for convenience in notation; remember, however, that whenever a subscript, such as ijk , represents the node number in three dimensions a corresponding superscript should indicate the element number under consideration.

$$\begin{aligned} \nabla \times \mathbf{V}^e = & (r_y^e \frac{\partial W^e}{\partial r} + s_y^e \frac{\partial W^e}{\partial s} + t_y^e \frac{\partial W^e}{\partial t} - r_z^e \frac{\partial V^e}{\partial r} - s_z^e \frac{\partial V^e}{\partial s} - t_z^e \frac{\partial V^e}{\partial t}) \mathbf{e}_x \\ & + (r_z^e \frac{\partial U^e}{\partial r} + s_z^e \frac{\partial U^e}{\partial s} + t_z^e \frac{\partial U^e}{\partial t} - r_x^e \frac{\partial W^e}{\partial r} - s_x^e \frac{\partial W^e}{\partial s} - t_x^e \frac{\partial W^e}{\partial t}) \mathbf{e}_y \\ & + (r_x^e \frac{\partial V^e}{\partial r} + s_x^e \frac{\partial V^e}{\partial s} + t_x^e \frac{\partial V^e}{\partial t} - r_y^e \frac{\partial U^e}{\partial r} - s_y^e \frac{\partial U^e}{\partial s} - t_y^e \frac{\partial U^e}{\partial t}) \mathbf{e}_z. \end{aligned}$$

The three components of the vorticity equal

$$\zeta_x^e = r_y^e \frac{\partial W^e}{\partial r} + s_y^e \frac{\partial W^e}{\partial s} + t_y^e \frac{\partial W^e}{\partial t} - r_z^e \frac{\partial V^e}{\partial r} - s_z^e \frac{\partial V^e}{\partial s} - t_z^e \frac{\partial V^e}{\partial t}, \quad (4.3.4a)$$

$$\zeta_y^e = r_z^e \frac{\partial U^e}{\partial r} + s_z^e \frac{\partial U^e}{\partial s} + t_z^e \frac{\partial U^e}{\partial t} - r_x^e \frac{\partial W^e}{\partial r} - s_x^e \frac{\partial W^e}{\partial s} - t_x^e \frac{\partial W^e}{\partial t}, \quad (4.3.4b)$$

and
$$\zeta_z^e = r_x^e \frac{\partial V^e}{\partial r} + s_x^e \frac{\partial V^e}{\partial s} + t_x^e \frac{\partial V^e}{\partial t} - r_y^e \frac{\partial U^e}{\partial r} - s_y^e \frac{\partial U^e}{\partial s} - t_y^e \frac{\partial U^e}{\partial t}. \quad (4.3.4c)$$

The x-vorticity evaluated at the local co-ordinate r_i, s_j, t_k appears as

$$\begin{aligned} (\zeta_x)^e_{ijk} = & (r_y)^e_{ijk} \frac{\partial \bar{W}^e}{\partial r}_{ijk} + (s_y)^e_{ijk} \frac{\partial \bar{W}^e}{\partial s}_{ijk} + (t_y)^e_{ijk} \frac{\partial \bar{W}^e}{\partial t}_{ijk} \\ & - (r_z)^e_{ijk} \frac{\partial \bar{V}^e}{\partial r}_{ijk} - (s_z)^e_{ijk} \frac{\partial \bar{V}^e}{\partial s}_{ijk} - (t_z)^e_{ijk} \frac{\partial \bar{V}^e}{\partial t}_{ijk}. \end{aligned} \quad (4.3.5)$$

The partial derivative with respect to the local co-ordinate, r , equals (see appendix A)

$$\frac{\partial}{\partial r}^e_{ijk} = \sum_{abc} D_{ia} \delta_{jb} \delta_{kc}. \quad (4.3.6)$$

Similar expressions exist for the s and t components. Substituting into (4.3.5)

gives (4.3.7)

$$\begin{aligned} (\zeta_x)^e_{ijk} = & \sum_{abc} [(r_y)^e_{ijk} D_{ia} \delta_{jb} \delta_{kc} + (s_y)^e_{ijk} \delta_{ia} D_{jb} \delta_{kc} + (t_y)^e_{ijk} \delta_{ia} \delta_{jb} D_{kc}] \bar{W}^e_{ijk} \\ & - \sum_{abc} [(r_z)^e_{ijk} D_{ia} \delta_{jb} \delta_{kc} + (s_z)^e_{ijk} \delta_{ia} D_{jb} \delta_{kc} + (t_z)^e_{ijk} \delta_{ia} \delta_{jb} D_{kc}] \bar{V}^e_{ijk}. \end{aligned}$$

Expressing the other vorticity components this way gives an equation for the vorticity vector at the local node (r_i, s_j, t_k) :

$$\begin{aligned} \tilde{\zeta}^e_{ijk} = & \sum_{abc} \left\{ [(r_y)^e_{ijk} D_{ia} \delta_{jb} \delta_{kc} + (s_y)^e_{ijk} \delta_{ia} D_{jb} \delta_{kc} + (t_y)^e_{ijk} \delta_{ia} \delta_{jb} D_{kc}] \bar{W}^e_{ijk} \right. \\ & - [(r_z)^e_{ijk} D_{ia} \delta_{jb} \delta_{kc} + (s_z)^e_{ijk} \delta_{ia} D_{jb} \delta_{kc} + (t_z)^e_{ijk} \delta_{ia} \delta_{jb} D_{kc}] \bar{V}^e_{ijk} \Big\} \mathbf{e}_x \\ & + \left\{ [(r_z)^e_{ijk} D_{ia} \delta_{jb} \delta_{kc} + (s_z)^e_{ijk} \delta_{ia} D_{jb} \delta_{kc} + (t_z)^e_{ijk} \delta_{ia} \delta_{jb} D_{kc}] \bar{U}^e_{ijk} \right. \\ & - [(r_x)^e_{ijk} D_{ia} \delta_{jb} \delta_{kc} + (s_x)^e_{ijk} \delta_{ia} D_{jb} \delta_{kc} + (t_x)^e_{ijk} \delta_{ia} \delta_{jb} D_{kc}] \bar{W}^e_{ijk} \Big\} \mathbf{e}_y \end{aligned} \quad (4.3.8)$$

$$+ \left[[(r_x)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_x)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_x)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{V}_{ijk}^e - [(r_y)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_y)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_y)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{U}_{ijk}^e \right] e_z \Big\}.$$

4.4 Spatial Discretization of Cross-Product of Velocity with Vorticity

The cross-product of the velocity with the vorticity appears as

$$\mathbf{V} \times \boldsymbol{\zeta} = (V_{\zeta_z} - W_{\zeta_y}) \mathbf{e}_x + (W_{\zeta_x} - U_{\zeta_z}) \mathbf{e}_y + (U_{\zeta_y} - V_{\zeta_x}) \mathbf{e}_z. \quad (4.4.1)$$

Using the discrete expressions for the velocity and vorticity gives

$$(\tilde{\mathbf{V}} \times \tilde{\boldsymbol{\zeta}})_{ijk}^e = \sum_{abc} \left\{ \begin{aligned} & \left[[(r_x)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_x)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_x)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{V}_{ijk}^e - [(r_y)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_y)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_y)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{U}_{ijk}^e \right] \tilde{V}_{ijk}^e \\ & - \left[[(r_z)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_z)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_z)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{U}_{ijk}^e - [(r_x)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_x)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_x)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{W}_{ijk}^e \right] \tilde{W}_{ijk}^e \Big] \mathbf{e}_x \\ & + \left[[(r_y)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_y)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_y)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{W}_{ijk}^e - [(r_z)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_z)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_z)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{V}_{ijk}^e \right] \tilde{W}_{ijk}^e \\ & - \left[[(r_x)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_x)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_x)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{V}_{ijk}^e - [(r_y)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_y)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_y)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{U}_{ijk}^e \right] \tilde{U}_{ijk}^e \Big] \mathbf{e}_y \\ & + \left[[(r_z)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_z)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_z)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{U}_{ijk}^e - [(r_x)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_x)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_x)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{W}_{ijk}^e \right] \tilde{U}_{ijk}^e \\ & - \left[[(r_y)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_y)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_y)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{W}_{ijk}^e - [(r_z)_{ijk}^e D_{ia} \delta_{jb} \delta_{kc} + (s_z)_{ijk}^e \delta_{ia} D_{jb} \delta_{kc} + (t_z)_{ijk}^e \delta_{ia} \delta_{jb} D_{kc}] \tilde{V}_{ijk}^e \right] \tilde{V}_{ijk}^e \Big] \mathbf{e}_z \Big\} \end{aligned} \right. \quad (4.4.2)$$

for the cross-product of the velocity with the vorticity at the local node (r_i, s_j, t_k) .

4.5 Summary

The equation governing the velocity after the pressure step equals

$$\begin{aligned} \tilde{\mathbf{V}}_{ijk}^{n+1} &= \tilde{\mathbf{V}}_{ijk}^n + B_0 \Delta t [(\mathbf{V} \times \tilde{\boldsymbol{\zeta}})_{ijk}^e + \mathbf{f}_{ijk}^e]^n \\ &+ B_1 \Delta t [(\mathbf{V} \times \tilde{\boldsymbol{\zeta}})_{ijk}^e + \mathbf{f}_{ijk}^e]^{n-1} + B_2 \Delta t [(\mathbf{V} \times \tilde{\boldsymbol{\zeta}})_{ijk}^e + \mathbf{f}_{ijk}^e]^{n-2}, \end{aligned} \quad (4.5.1)$$

where the terms $(\mathbf{V} \times \tilde{\boldsymbol{\zeta}})_{ijk}^e$ appear in (4.4.2). This explicit relation for the

unknown velocity coefficients at time step $n+1$ depends on known quantities from the previous step, denoted by the superscript n . Its solution does not involve inverting the stiffness matrix; unfortunately, however, this simplicity comes with a concomitant loss of accuracy—the collocation scheme searches for the solution with a measurement device tolerating first-order errors in time.

CHAPTER V

PRESSURE STEP

5.1 Variational Approach

According to §3.4, the governing differential relation for the pressure step equals

$$\frac{\nabla \cdot \tilde{\mathbf{V}}^{n+1}}{\Delta t} = \nabla \cdot \nabla P. \quad (5.1.1)$$

This represents an elliptic, Poisson equation; consequently, a corresponding variational form exists. For the moment, assume that the functional whose Euler-Lagrange equation yields (5.1.1) equals

$$J[P] = \int_{\Omega} \left[-\frac{1}{2} (\nabla P \cdot \nabla P) \Delta t + \tilde{\mathbf{V}}^{n+1} \cdot \nabla P \right] dV. \quad (5.1.2)$$

The standard boundary conditions accompanying a functional of this type equal

$$\mathbf{n} \cdot \frac{\partial F}{\partial \nabla P} = 0, \quad (5.1.3)$$

where F equals the integrand of the functional. Applying this boundary condition formula to the functional shown in (5.1.2) yields

$$-\mathbf{n} \cdot \nabla P \Delta t + \mathbf{n} \cdot \tilde{\mathbf{V}}^{n+1} = 0. \quad (5.1.4)$$

According to the derivation in §3.4 the appropriate boundary conditions for the pressure step equal

$$-\mathbf{n} \cdot \nabla P \Delta t + \mathbf{n} \cdot \tilde{\mathbf{V}}^{n+1} = \mathbf{n} \cdot \check{\mathbf{V}}^{n+1}, \quad (5.1.5)$$

which does not correspond to that shown in (5.1.4), since an additional $\mathbf{n} \cdot \check{\mathbf{V}}^{n+1}$ exists on the right-hand side; therefore, we must add a boundary integral to our functional. Thus, the functional satisfying the appropriate boundary conditions and the governing pressure step relation equals

$$J[P] = \int_{\Omega} \left[-\frac{1}{2} (\nabla P \cdot \nabla P) \Delta t + \tilde{\mathbf{V}}^{n+1} \cdot \nabla P \right] dV - \int_{\partial\Omega} P (\mathbf{n} \cdot \check{\mathbf{V}}^{n+1}) d\sigma. \quad (5.1.6)$$

Applying the Euler-Lagrange equation to this functional yields (5.1.1) with boundary conditions (5.1.5). A demonstration of this follows.

Up until this point, we accepted the validity of the functional shown in (5.1.6) *prima facie*. We must show that the extremum of this functional does indeed yield the differential relation and boundary conditions for the pressure step. We begin by considering the variation of $J[P]$ with respect to P :

$$\delta J[P] = \int_{\Omega} [-\nabla P \cdot \nabla(\delta P)\Delta t + \tilde{V}^{n+1} \cdot \nabla(\delta P)] dV - \int_{\partial\Omega} (\mathbf{n} \cdot \tilde{V}^{n+1}) \delta P d\sigma. \quad (5.1.7)$$

Rearranging gives

$$\begin{aligned} \delta J[P] = \int_{\Omega} [-\nabla \cdot (\nabla P \delta P)\Delta t + \delta P \nabla \cdot \nabla P \Delta t + \nabla \cdot (\tilde{V}^{n+1} \delta P) - \delta P \nabla \cdot \tilde{V}^{n+1}] dV \\ - \int_{\partial\Omega} (\mathbf{n} \cdot \tilde{V}^{n+1}) \delta P d\sigma. \end{aligned} \quad (5.1.8)$$

Employing Gauss' divergence theorem, we transform the first and third volume integrals into surface integrals giving

$$\begin{aligned} \delta J[P] = \int_{\Omega} [\nabla \cdot \nabla P \Delta t - \nabla \cdot \tilde{V}^{n+1}] \delta P dV \\ + \int_{\partial\Omega} [-\mathbf{n} \cdot \nabla P \Delta t + \mathbf{n} \cdot \tilde{V}^{n+1} - \mathbf{n} \cdot \tilde{V}^{n+1}] \delta P d\sigma. \end{aligned} \quad (5.1.9)$$

An extremum of $J[P]$ occurs when this variation equals zero. Since the variation of P on the boundary of the domain does not depend on its variation within the boundary, the extremum occurs when both

$$\nabla \cdot \nabla P \Delta t - \nabla \cdot \tilde{V}^{n+1} = 0, \quad (5.1.10)$$

within the volume of the domain, and

$$-\mathbf{n} \cdot \nabla P \Delta t + \mathbf{n} \cdot \tilde{V}^{n+1} - \mathbf{n} \cdot \tilde{V}^{n+1} = 0, \quad (5.1.11)$$

on the boundary, are satisfied simultaneously. We see that these equations equal the governing equation and boundary conditions. Thus, the variation of the functional given by (5.1.6) yields the Poisson equation shown in (5.1.1) with boundary conditions (5.1.5).

5.2 Representation in Local Co-ordinates

We must transform the functional in (5.1.6) from the global x,y,z co-ordinate system to the local r,s,t system. The corresponding functional

representation for a single element, designated by the superscript e , in local co-ordinates equals

$$J[P]^e = \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \left[-\frac{1}{2} (\nabla P \cdot \nabla P) \Delta t + \tilde{V} \cdot \nabla P \right]^e |\det[J^e]| dr ds dt - \sum_{p=1}^6 \int_{-1}^1 \int_{-1}^1 P^e(\mathbf{n} \cdot \tilde{V}^e) dA^p, \quad (5.2.1)$$

where we drop the superscript indicating the time step number and replace it by a superscript indicating element number. (Consult appendix B for details of the volume element conversion from global to local co-ordinates.) The surface integral contains expressions for the summation over the six faces of each element. We will consider the details of these terms later.

This functional, approximated by expressing it in terms of the expansion polynomials, for example, $P^e \approx \sum_{abc} \tilde{P}_{abc}^e \psi_a(r) \psi_b(s) \psi_c(t)$, appears as

$$J[P]^e \approx \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \sum_{abc} \left[-\frac{1}{2} \nabla_{abc}^e \tilde{P}_{abc}^e \cdot \nabla_{abc}^e \tilde{P}_{abc}^e \Delta t + \tilde{V}_{abc}^e \cdot \nabla_{abc}^e \tilde{P}_{abc}^e \right] \psi_a(r) \psi_b(s) \psi_c(t) |\det[J^e]|_{abc} dr ds dt - \sum_{p=1}^6 I_p^e. \quad (5.2.2)$$

A brief explanation of the accompanying notation seems appropriate. The subscript abc refers to the node r_a, s_b, t_c , while the tilde refers to the corresponding unknown expansion coefficients. We postpone treatment of the surface integral, conveniently expressed in the interim as $\sum_{p=1}^6 I_p^e$, until §5.3.

Many of the following numerical minutiae receive a more thorough treatment in the following chapter dealing with the viscous step. The gradient operator in global co-ordinates equals

$$\nabla_{abc}^e \tilde{P}_{abc}^e = \frac{\partial \tilde{P}_{abc}^e}{\partial x} \mathbf{e}_x + \frac{\partial \tilde{P}_{abc}^e}{\partial y} \mathbf{e}_y + \frac{\partial \tilde{P}_{abc}^e}{\partial z} \mathbf{e}_z. \quad (5.2.3)$$

In the local co-ordinate system this operator equals

$$\nabla_{abc}^e \tilde{P}_{abc}^e = \left[\frac{\partial \tilde{P}_{abc}^e}{\partial r} (r_x^e)_{abc} + \frac{\partial \tilde{P}_{abc}^e}{\partial s} (s_x^e)_{abc} + \frac{\partial \tilde{P}_{abc}^e}{\partial t} (t_x^e)_{abc} \right] \mathbf{e}_x + \quad (5.2.4)$$

$$\begin{aligned} & \left[\frac{\partial \tilde{P}_{abc}^e}{\partial r} (r_y^e)_{abc} + \frac{\partial \tilde{P}_{abc}^e}{\partial s} (s_y^e)_{abc} + \frac{\partial \tilde{P}_{abc}^e}{\partial t} (t_y^e)_{abc} \right] e_y + \\ & \left[\frac{\partial \tilde{P}_{abc}^e}{\partial r} (r_z^e)_{abc} + \frac{\partial \tilde{P}_{abc}^e}{\partial s} (s_z^e)_{abc} + \frac{\partial \tilde{P}_{abc}^e}{\partial t} (t_z^e)_{abc} \right] e_z. \end{aligned}$$

Introducing expansions for the local partial derivatives according to (6.3.5) through (6.3.7) gives

$$\begin{aligned} \nabla_{abc}^e \tilde{P}_{abc}^e = & \quad (5.2.5) \\ \sum_{ijk} & \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_x + \right. \\ & [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_y + \\ & \left. [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_z \right] \tilde{P}_{ijk}^e. \end{aligned}$$

The inner product of this term with a term of similar form appears as

$$\begin{aligned} \nabla_{abc}^e \tilde{P}_{abc}^e \cdot \nabla_{abc}^e \tilde{P}_{abc}^e = & \quad (5.2.6) \\ \sum_{ijk} & \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_x + \right. \\ & [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_y + \\ & \left. [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_z \right] \tilde{P}_{ijk}^e \cdot \\ \sum_{lmn} & \left[[(r_x^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_x^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_x^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] e_x + \right. \\ & [(r_y^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_y^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_y^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] e_y + \\ & \left. [(r_z^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_z^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_z^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] e_z \right] \tilde{P}_{lmn}^e. \end{aligned}$$

Performing the inner product gives

$$\begin{aligned} \nabla_{abc}^e \tilde{P}_{abc}^e \cdot \nabla_{abc}^e \tilde{P}_{abc}^e = & \sum_{ijk} \sum_{lmn} \tilde{P}_{ijk}^e \tilde{P}_{lmn}^e \quad (5.2.7) \\ & \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \right. \\ & [(r_x^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_x^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_x^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\ & [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\ & [(r_y^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_y^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_y^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\ & [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\ & \left. [(r_z^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_z^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_z^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] \right]. \end{aligned}$$

Introducing these expressions into (5.2.2) gives

$$\begin{aligned}
J[P]^e \approx & \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \sum_{abc} \psi_a(r) \psi_b(s) \psi_c(t) |\det[J^e]|_{abc} \left[-\frac{1}{2} \sum_{ijk} \sum_{lmn} \tilde{P}_{ijk}^e \tilde{P}_{lmn}^e \Delta t \right. \\
& \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \right. \\
& [(r_x^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_x^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_x^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_y^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_y^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_y^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\
& \left. \left. [(r_z^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_z^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_z^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] \right] \right. \\
& + \tilde{V}_{abc}^e \cdot \sum_{ijk} \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_x + \right. \\
& [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_y + \\
& \left. [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_z \right] \tilde{P}_{ijk}^e \Big] dr ds dt \\
& - \sum_{p=1}^6 I_p^e. \tag{5.2.8}
\end{aligned}$$

Evaluating the integrals by introducing $w_a = \int_{-1}^1 \psi_a(r) dr$ according to (1.5.16)

gives

$$\begin{aligned}
J[P]^e \approx & -\frac{1}{2} \sum_{abc} \sum_{ijk} \sum_{lmn} \tilde{P}_{ijk}^e \tilde{P}_{lmn}^e \Delta t w_a w_b w_c |\det[J^e]|_{abc} \\
& \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \right. \\
& [(r_x^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_x^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_x^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_y^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_y^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_y^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\
& \left. [(r_z^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_z^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_z^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] \right] \\
& + \sum_{abc} \tilde{V}_{abc}^e \cdot \sum_{ijk} \tilde{P}_{ijk}^e w_a w_b w_c |\det[J^e]|_{abc} \\
& \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_x + \right. \\
& [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_y + \\
& \left. [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_z \right] \\
& - \sum_{p=1}^6 I_p^e. \tag{5.2.9}
\end{aligned}$$

Excluding the surface integral, this represents the governing functional in terms of the local co-ordinates.

5.3 Surface Integral

The surface integral,

$$\sum_{p=1}^6 I^{pe} = \sum_{p=1}^6 \int_{-1}^1 \int_{-1}^1 P^e(\mathbf{n} \cdot \tilde{\mathbf{V}}^e) dA^p, \quad (5.3.1)$$

contains contributions from each of the six sides of each element. We must express it in terms of the unknown expansion coefficients in the local (r,s,t) co-ordinate system. Rearranging (5.3.1) by combining the surface unit normal vector, \mathbf{n} , with the differential area, dA , gives

$$\sum_{p=1}^6 I^{pe} = \sum_{p=1}^6 \int_{-1}^1 \int_{-1}^1 P^e \tilde{\mathbf{V}}^e \cdot d\mathbf{A}^p. \quad (5.3.2)$$

Introducing these expressions for each of the six faces on the local element gives

$$\begin{aligned} \sum_{p=1}^6 I^{pe} = & \\ & - \int_{-1}^1 \int_{-1}^1 P^e \tilde{\mathbf{V}}^e \cdot (x_3 \mathbf{e}_x + y_3 \mathbf{e}_y + z_3 \mathbf{e}_z) dr ds \\ & + \int_{-1}^1 \int_{-1}^1 P^e \tilde{\mathbf{V}}^e \cdot (x_2 \mathbf{e}_x + y_2 \mathbf{e}_y + z_2 \mathbf{e}_z) dr dt \\ & + \int_{-1}^1 \int_{-1}^1 P^e \tilde{\mathbf{V}}^e \cdot (x_3 \mathbf{e}_x + y_3 \mathbf{e}_y + z_3 \mathbf{e}_z) dr ds \\ & - \int_{-1}^1 \int_{-1}^1 P^e \tilde{\mathbf{V}}^e \cdot (x_2 \mathbf{e}_x + y_2 \mathbf{e}_y + z_2 \mathbf{e}_z) dr dt \\ & - \int_{-1}^1 \int_{-1}^1 P^e \tilde{\mathbf{V}}^e \cdot (x_1 \mathbf{e}_x + y_1 \mathbf{e}_y + z_1 \mathbf{e}_z) ds dt \\ & + \int_{-1}^1 \int_{-1}^1 P^e \tilde{\mathbf{V}}^e \cdot (x_1 \mathbf{e}_x + y_1 \mathbf{e}_y + z_1 \mathbf{e}_z) ds dt, \end{aligned} \quad (5.3.3)$$

where we expressed the area vectors shown in (5.3.2) in terms of their component parts with the assistance of §A.7 in appendix A. Introducing the expansion polynomials into these surface integrals gives

$$\begin{aligned} \sum_{p=1}^6 I^{pe} \approx & \\ & - \int_{-1}^1 \int_{-1}^1 \sum_{ab} \tilde{P}_{ab1}^e \tilde{\mathbf{V}}_{ab1}^e \cdot (x_3 \mathbf{e}_x + y_3 \mathbf{e}_y + z_3 \mathbf{e}_z)_{ab1} \psi_a(r) \psi_b(s) dr ds \\ & + \int_{-1}^1 \int_{-1}^1 \sum_{ac} \tilde{P}_{ac2}^e \tilde{\mathbf{V}}_{ac2}^e \cdot (x_2 \mathbf{e}_x + y_2 \mathbf{e}_y + z_2 \mathbf{e}_z)_{ac2} \psi_a(r) \psi_c(t) dr dt \end{aligned} \quad (5.3.4)$$

$$\begin{aligned}
& + \int_{-1}^1 \int_{-1}^1 \sum_{ab} \tilde{P}_{ab2}^e \tilde{V}_{ab2}^e \cdot (x_3 e_x + y_3 e_y + z_3 e_z)_{ab2} \psi_a(r) \psi_b(s) dr ds \\
& - \int_{-1}^1 \int_{-1}^1 \sum_{ac} \tilde{P}_{a1c}^e \tilde{V}_{a1c}^e \cdot (x_2 e_x + y_2 e_y + z_2 e_z)_{a1c} \psi_a(r) \psi_c(t) dr dt \\
& - \int_{-1}^1 \int_{-1}^1 \sum_{bc} \tilde{P}_{1bc}^e \tilde{V}_{1bc}^e \cdot (x_1 e_x + y_1 e_y + z_1 e_z)_{1bc} \psi_b(s) \psi_c(t) ds dt \\
& + \int_{-1}^1 \int_{-1}^1 \sum_{bc} \tilde{P}_{2bc}^e \tilde{V}_{2bc}^e \cdot (x_1 e_x + y_1 e_y + z_1 e_z)_{2bc} \psi_b(s) \psi_c(t) ds dt.
\end{aligned}$$

Evaluating the integrals using $w_a = \int_{-1}^1 \psi_a(r) dr$ gives

$$\begin{aligned}
& \sum_{p=1}^6 I^p e \approx \quad (5.3.5) \\
& - \sum_{ab} \tilde{P}_{ab1}^e \tilde{V}_{ab1}^e \cdot (x_3 e_x + y_3 e_y + z_3 e_z)_{ab1} w_a w_b \\
& + \sum_{ac} \tilde{P}_{a2c}^e \tilde{V}_{a2c}^e \cdot (x_2 e_x + y_2 e_y + z_2 e_z)_{a2c} w_a w_c \\
& + \sum_{ab} \tilde{P}_{ab2}^e \tilde{V}_{ab2}^e \cdot (x_3 e_x + y_3 e_y + z_3 e_z)_{ab2} w_a w_b \\
& - \sum_{ac} \tilde{P}_{a1c}^e \tilde{V}_{a1c}^e \cdot (x_2 e_x + y_2 e_y + z_2 e_z)_{a1c} w_a w_c \\
& - \sum_{bc} \tilde{P}_{1bc}^e \tilde{V}_{1bc}^e \cdot (x_1 e_x + y_1 e_y + z_1 e_z)_{1bc} w_b w_c \\
& + \sum_{bc} \tilde{P}_{2bc}^e \tilde{V}_{2bc}^e \cdot (x_1 e_x + y_1 e_y + z_1 e_z)_{2bc} w_b w_c.
\end{aligned}$$

Finally, performing the inner product using $\tilde{V}_{abc}^e = \tilde{U}_{abc}^e e_x + \tilde{V}_{abc}^e e_y + \tilde{W}_{abc}^e e_z$ gives

$$\begin{aligned}
& \sum_{p=1}^6 I^p e \approx \quad (5.3.6) \\
& - \sum_{ab} \tilde{P}_{ab1}^e (\tilde{U}_{ab1}^e x_3 + \tilde{V}_{ab1}^e y_3 + \tilde{W}_{ab1}^e z_3)_{ab1} w_a w_b \\
& + \sum_{ac} \tilde{P}_{a2c}^e (\tilde{U}_{a2c}^e x_2 + \tilde{V}_{a2c}^e y_2 + \tilde{W}_{a2c}^e z_2)_{a2c} w_a w_c \\
& + \sum_{ab} \tilde{P}_{ab2}^e (\tilde{U}_{ab2}^e x_3 + \tilde{V}_{ab2}^e y_3 + \tilde{W}_{ab2}^e z_3)_{ab2} w_a w_b \\
& - \sum_{ac} \tilde{P}_{a1c}^e (\tilde{U}_{a1c}^e x_2 + \tilde{V}_{a1c}^e y_2 + \tilde{W}_{a1c}^e z_2)_{a1c} w_a w_c \\
& - \sum_{bc} \tilde{P}_{1bc}^e (\tilde{U}_{1bc}^e x_1 + \tilde{V}_{1bc}^e y_1 + \tilde{W}_{1bc}^e z_1)_{1bc} w_b w_c \\
& + \sum_{bc} \tilde{P}_{2bc}^e (\tilde{U}_{2bc}^e x_1 + \tilde{V}_{2bc}^e y_1 + \tilde{W}_{2bc}^e z_1)_{2bc} w_b w_c.
\end{aligned}$$

5.4 Variation of the Functional

All of the pieces corresponding to the terms in the governing functional exist in terms of the local co-ordinates and expansion functions and coefficients. Substituting (5.3.6) into (5.2.9) and performing the remaining inner product gives

$$\begin{aligned}
 J[P]^e \approx & -\frac{1}{2} \sum_{abc} \sum_{ijk} \sum_{lmn} \bar{P}_{ijk}^e \bar{P}_{lmn}^e \Delta t w_a w_b w_c |\det[J^e]|_{abc} \\
 & \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \right. \\
 & [(r_x^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_x^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_x^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\
 & [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\
 & [(r_y^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_y^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_y^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\
 & [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\
 & \left. [(r_z^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_z^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_z^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] \right] \\
 & + \sum_{abc} \sum_{ijk} \bar{P}_{ijk}^e w_a w_b w_c |\det[J^e]|_{abc} \quad (5.4.1) \\
 & \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \tilde{U}_{abc}^e + \right. \\
 & [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \tilde{V}_{abc}^e + \\
 & \left. [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \tilde{W}_{abc}^e \right] \\
 & - \sum_{ab} \bar{P}_{ab1}^e (\tilde{U}_{ab1}^e x_3 + \tilde{V}_{ab1}^e y_3 + \tilde{W}_{ab1}^e z_3)_{ab1} w_a w_b \\
 & + \sum_{ac} \bar{P}_{a2c}^e (\tilde{U}_{a2c}^e x_2 + \tilde{V}_{a2c}^e y_2 + \tilde{W}_{a2c}^e z_2)_{a2c} w_a w_c \\
 & + \sum_{ab} \bar{P}_{ab2}^e (\tilde{U}_{ab2}^e x_3 + \tilde{V}_{ab2}^e y_3 + \tilde{W}_{ab2}^e z_3)_{ab2} w_a w_b \\
 & - \sum_{ac} \bar{P}_{a1c}^e (\tilde{U}_{a1c}^e x_2 + \tilde{V}_{a1c}^e y_2 + \tilde{W}_{a1c}^e z_2)_{a1c} w_a w_c \\
 & - \sum_{bc} \bar{P}_{1bc}^e (\tilde{U}_{1bc}^e x_1 + \tilde{V}_{1bc}^e y_1 + \tilde{W}_{1bc}^e z_1)_{1bc} w_b w_c \\
 & + \sum_{bc} \bar{P}_{2bc}^e (\tilde{U}_{2bc}^e x_1 + \tilde{V}_{2bc}^e y_1 + \tilde{W}_{2bc}^e z_1)_{2bc} w_b w_c.
 \end{aligned}$$

The extremum of $J[P]$, or the variation $\partial J[P]/\partial P$, equals

$$\begin{aligned}
\partial J[P]^e / \partial P \approx & - \sum_{abc} \sum_{ijk} \bar{P}_{ijk}^e \Delta t w_a w_b w_c |\det[J^e]|_{abc} \\
& \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \right. \\
& [(r_x^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_x^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_x^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_y^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_y^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_y^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\
& \left. [(r_z^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_z^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_z^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] \right] \\
& + \sum_{abc} w_a w_b w_c |\det[J^e]|_{abc} \quad (5.4.2)
\end{aligned}$$

$$\begin{aligned}
& \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \tilde{U}_{abc}^e + \right. \\
& [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \tilde{V}_{abc}^e + \\
& \left. [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \tilde{W}_{abc}^e \right] \\
& - \sum_{ab} (\tilde{U}_{ab1}^e x_3 + \tilde{V}_{ab1}^e y_3 + \tilde{W}_{ab1}^e z_3)_{ab1} w_a w_b \\
& + \sum_{ac} (\tilde{U}_{a2c}^e x_2 + \tilde{V}_{a2c}^e y_2 + \tilde{W}_{a2c}^e z_2)_{a2c} w_a w_c \\
& + \sum_{ab} (\tilde{U}_{ab2}^e x_3 + \tilde{V}_{ab2}^e y_3 + \tilde{W}_{ab2}^e z_3)_{ab2} w_a w_b \\
& - \sum_{ac} (\tilde{U}_{a1c}^e x_2 + \tilde{V}_{a1c}^e y_2 + \tilde{W}_{a1c}^e z_2)_{a1c} w_a w_c \\
& - \sum_{bc} (\tilde{U}_{1bc}^e x_1 + \tilde{V}_{1bc}^e y_1 + \tilde{W}_{1bc}^e z_1)_{1bc} w_b w_c \\
& + \sum_{bc} (\tilde{U}_{2bc}^e x_1 + \tilde{V}_{2bc}^e y_1 + \tilde{W}_{2bc}^e z_1)_{2bc} w_b w_c.
\end{aligned}$$

The middle term in (5.4.2) may appear more conveniently as

$$\begin{aligned}
& \sum_{abc} w_a w_b w_c |\det[J^e]|_{abc} \quad (5.4.3) \\
& \left[[(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \tilde{U}_{abc}^e + \right. \\
& [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \tilde{V}_{abc}^e + \\
& \left. [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \tilde{W}_{abc}^e \right]
\end{aligned}$$

$$\equiv \sum_{abc} \nabla_{abcijk}^e \cdot \tilde{V}_{abc}^e w_a w_b w_c |\det[J^e]|_{abc}$$

where the divergence operator† equals

$$\nabla_{abcijk}^e \equiv \quad (5.4.4)$$

$$\begin{aligned} & [(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_x + \\ & [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_y + \\ & [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] e_z. \end{aligned}$$

Introducing the quantity Π_{lmnabc}^e , defined by

$$\Pi_{lmnabc}^e \equiv -|\det[J^e]|_{abc} w_a w_b w_c \delta_{la} \delta_{mb} \delta_{nc}, \quad (5.4.5)$$

into (5.4.3) gives

$$\sum_{abc} \nabla_{abcijk}^e \cdot \tilde{V}_{abc}^e w_a w_b w_c |\det[J^e]|_{abc} = - \sum_{lmn} \sum_{abc} \nabla_{lmnijk}^e \cdot \Pi_{lmnabc}^e \tilde{V}_{abc}^e, \quad (5.4.6)$$

for the middle term in (5.4.2). The free set of indices in this expression equal ijk , while those in the first term in (5.4.2) equal lmn . Rearranging the indices gives an equivalent form for the right-hand side of (5.4.6), written as

$$\sum_{ijk} \sum_{abc} \nabla_{ijklmn}^e \cdot \Pi_{ijkabc}^e \tilde{V}_{abc}^e. \quad (5.4.7)$$

The extremum of $J[P]$ occurs when the expression in (5.4.2) equals zero.

Substituting (5.4.7) for the middle term and, setting $\delta J[P]/\delta P=0$ gives

$$\sum_{ijk} \Lambda_{lmnijk}^e \tilde{P}_{ijk}^e \Delta t = - \sum_{ijk} \sum_{abc} \nabla_{ijklmn}^e \cdot \Pi_{ijkabc}^e \tilde{V}_{abc}^e + \check{S}^e, \quad (5.4.8)$$

where the surface integral appears as

$$\check{S}^e = \quad (5.4.9)$$

$$\begin{aligned} & - \sum_{ab} (\tilde{U}_{ab1x3}^e + \tilde{V}_{ab1y3}^e + \tilde{W}_{ab1z3}^e)_{ab1} w_a w_b \\ & + \sum_{ac} (\tilde{U}_{a2cx2}^e + \tilde{V}_{a2cy2}^e + \tilde{W}_{a2cz2}^e)_{a2c} w_a w_c \end{aligned}$$

†The term $\nabla_{abcijk} \cdot V_{abc}$, obtained from the expression $V \cdot \nabla$ does not equal the divergence of velocity. We write the divergence of velocity $\nabla \cdot V$ as $\nabla_{abcijk} V_{ijk}$. Hence, the order of indices is important.

$$\begin{aligned}
& + \sum_{ab} (\tilde{U}_{ab2}^e x_3 + \tilde{V}_{ab2}^e y_3 + \tilde{W}_{ab2}^e z_3)_{ab2} w_a w_b \\
& - \sum_{ac} (\tilde{U}_{a1c}^e x_2 + \tilde{V}_{a1c}^e y_2 + \tilde{W}_{a1c}^e z_2)_{a1c} w_a w_c \\
& - \sum_{bc} (\tilde{U}_{1bc}^e x_1 + \tilde{V}_{1bc}^e y_1 + \tilde{W}_{1bc}^e z_1)_{1bc} w_b w_c \\
& + \sum_{bc} (\tilde{U}_{2bc}^e x_1 + \tilde{V}_{2bc}^e y_1 + \tilde{W}_{2bc}^e z_1)_{2bc} w_b w_c,
\end{aligned}$$

and the quantity Λ_{mnijk}^e as

$$\begin{aligned}
\Lambda_{mnijk}^e = \sum_{abc} w_a w_b w_c |\det[J^e]|_{abc} \Big[& \quad (5.4.10) \\
& [(r_x^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_x^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_x^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_x^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_y^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_y^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_y^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_y^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_z^e)_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_z^e)_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_z^e)_{abc} \delta_{al} \delta_{bm} D_{cn}] \Big].
\end{aligned}$$

5.5 Solution for Pressure

Equation (5.4.8) applies to a single element. Adding the contributions from all elements gives

$$\sum_{e=1}^E \sum_{ijk} \Lambda_{mnijk}^e \bar{P}_{ijk}^e \Delta t = \sum_{e=1}^E \sum_{ijk} \sum_{abc} \nabla_{ijklmn}^e \cdot \Pi_{ijkabc}^e \tilde{V}_{abc}^e + \sum_{e=1}^E \check{S}^e. \quad (5.5.1)$$

In this expression, the pressure coefficients, \bar{P}_{ijk}^e , remain unknown; the velocity coefficients, \tilde{V}_{abc}^e , known from the non-linear step; and the surface integral unknown, since it contains unknown velocity coefficients \tilde{V}_{abc}^e . By summing over all elements, and taking advantage of the continuity of the velocity on the faces shared between elements, we greatly simplify the expression for the surface integral. Since the surface integrals contain velocities and not derivatives of velocity, and, since the velocity remains continuous throughout the domain, the

terms cancel on faces shared between two elements. Thus the summation over all elements yields a contribution from only those elements on the boundary of the domain. Unfortunately, the surface integral contains unknowns which represent the velocity after the pressure step. Hence, (5.5.1) contains two unknowns: pressure \tilde{P}_{ijk}^e and velocity $\tilde{\mathbf{V}}_{ijk}^e$. Along surfaces where we specify essential boundary conditions on velocity, the surface integral depends on known quantities; along surfaces where we specify natural boundary conditions, the velocity, $\tilde{\mathbf{V}}_{ijk}^e$, remains unknown. We may circumvent this problem by approximating the surface integral of $\mathbf{n} \cdot \tilde{\mathbf{V}}$ along natural boundaries by $\mathbf{n} \cdot \bar{\mathbf{V}}$, since we know $\bar{\mathbf{V}}$ from the non-linear step. However, since $\bar{\mathbf{V}}$ does not satisfy boundary conditions, a significant error may accrue from these integrals; furthermore, these integrals over the boundaries where both natural and essential conditions occur may require extensive computational time. Therefore, we use an entirely different technique for the surface integral expression.

Since $\sum_{e=1}^E \check{S}^e$ represents the net flux of velocity leaving the domain, $\iint_{\partial\Omega} (\mathbf{n} \cdot \mathbf{V}) dA$, we choose to compute the integral of $\mathbf{n} \cdot \bar{\mathbf{V}}$ over the inlet and exit boundaries and apply the difference of these terms to the exit velocity in the form of a correction. Hence, no longer do we satisfy (5.5.1) exactly at each of the nodal points. Instead, (5.5.1) holds only in a "global" sense. We approximate the surface integral by

$$\begin{aligned} \sum_{e=1}^E \check{S}^e &\approx \bar{\mathbf{V}}_{\text{out}} \cdot \mathbf{n} A_{\text{out}} \\ &= \int_{\partial\Omega_{\text{in}}} \mathbf{n} \cdot \bar{\mathbf{V}} d\sigma + \int_{\partial\Omega_{\text{out}}} \mathbf{n} \cdot \bar{\mathbf{V}} d\sigma, \end{aligned} \quad (5.5.2)$$

where $\bar{\mathbf{V}}_{\text{out}}$ equals the average outflow velocity correction and A_{out} equals the outflow area. The velocity correction applies to the velocity after the non-linear

step according to

$$(\tilde{\tilde{V}}_{ijk}^e)_{\text{corrected}} = \tilde{\tilde{V}}_{ijk}^e - \tilde{V}_{\text{out}}, \quad (5.5.3)$$

where node ijk and element e correspond to those nodes located along the exit portion of the domain, $\tilde{\tilde{V}}_{ijk}^e$ represents the known velocity after the non-linear step, and \tilde{V}_{out} the average velocity from (5.5.2). We use this corrected velocity in (5.5.1) in place of the original uncorrected velocity, and we drop the surface integral. The final form equals

$$\sum_{e=1}^E \sum_{ijk} A_{lmnijk}^e \tilde{P}_{ijk}^e \Delta t = \sum_{e=1}^E \sum_{ijk} \sum_{abc} \nabla_{ijklmn}^e \cdot \Pi_{ijkabc}^e (\tilde{\tilde{V}}_{abc}^e)_{\text{corrected}}.$$

Thus, we achieve the standard, linear form, $Ax=B$, for the unknown pressure coefficients. After computing the pressure, the velocity after the pressure step results from

$$\tilde{\tilde{V}}_{ijk}^e = \tilde{\tilde{V}}_{ijk}^e - \nabla_{ijk}^e \tilde{P}_{ijk}^e \Delta t, \quad (5.5.5)$$

equivalent to the discretized form of (3.2.2) applied at node ijk of element e .

Incidentally, a proviso must accompany quantities obtained from expressions with derivatives, such as (5.5.5). Since only the variables appearing in the essential boundary conditions remain continuous across elements, and not their derivatives, the gradient of pressure contains different values at the intersection between two elements—one value from each of the two elements. Since only one value may exist at any point in the global numbering scheme, before equations such as (5.5.5) get solved, we must combine the two values for ∇P at node ijk by taking the average value from the two elements. This seems innocuous enough; unfortunately, we break the zero divergence rule on $\tilde{\tilde{V}}_{ijk}^e$ in the process. This may induce important errors in certain problems.

CHAPTER VI

VISCOUS STEP

6.1 Variational Approach

The governing differential relation for the viscous step equals Helmholtz's equation, given by

$$\nabla^2 \phi - \lambda^2 \phi = F, \text{ in } \Omega. \quad (6.1.1)$$

We employ techniques from calculus of variations to generate a matrix expression for the unknown expansion coefficients ϕ_{ijk} . The goal remains finding a functional yielding Helmholtz's equation after application of the Euler-Lagrange formula. Assume for the moment, that the functional whose Euler-Lagrange equation corresponds to (6.1.1) with homogeneous boundary conditions given by

$$\alpha \phi + \beta (\mathbf{n} \cdot \nabla) \phi = 0, \text{ on } \partial \Omega, \quad (6.1.3)$$

equals

$$J[\phi] = \int_{\Omega} [-\frac{1}{2} \text{grad} \phi : \text{grad} \phi - \frac{1}{2} \lambda^2 \phi \cdot \phi - \phi \cdot F] dV. \quad (6.1.2)$$

This functional applies to domains with rigid boundaries. In fluid dynamics, both homogeneous and non-homogeneous boundary conditions arise. In general, the two possible types of non-homogeneous boundary conditions equal Dirichlet (essential) when $\beta=0$, given by

$$\phi = a, \quad (6.1.4)$$

and Neumann (natural) when $\alpha=0$, given by

$$(\mathbf{n} \cdot \nabla) \phi = g. \quad (6.1.5)$$

We may incorporate these non-homogeneous boundary conditions in the standard functional by adding a boundary integral.

Since ϕ must remain fixed along surfaces containing non-homogeneous Dirichlet boundary conditions according to (6.1.4), the variation in ϕ , written

as $\phi^* = \phi + \epsilon\psi$, must equal ϕ . In other words, we impose

$$\psi(\partial\Omega) = 0 \quad (6.1.6)$$

on surfaces with Dirichlet boundary conditions. We impose no restrictions on ψ , along boundaries with natural conditions. Instead, the natural or free boundary, where ϕ may vary, requires the standard constraint, $\mathbf{n} \cdot \partial F / \partial(\text{grad}\phi) = 0$, where F equals the integrand of the functional. The result, after applying this condition to the functional given in (6.1.2), equals $\mathbf{n} \cdot \text{grad}\phi = 0$, which does not satisfy the non-homogeneous natural boundary conditions. We overcome this problem by adding a surface integral to the functional giving

$$J[\phi] = \int_{\Omega} [-\frac{1}{2} \text{grad}\phi : \text{grad}\phi - \frac{1}{2} \lambda^2 \phi \cdot \phi - \phi \cdot F] dV + \int_{\partial\Omega^n} \phi \cdot \mathbf{g} d\sigma, \quad (6.1.7)$$

where $\partial\Omega^n$ represents the surface containing natural boundary conditions. The variation of the surface integral contributes a term, which when combined with $\mathbf{n} \cdot \partial F / \partial(\text{grad}\phi)$, yields the proper non-homogeneous natural boundary conditions. Until now, we accepted the claim that the functional shown in (6.1.7) yields Helmholtz's equation with appropriate boundary conditions without proof. We must show that the extremum of this functional does indeed yield Helmholtz's equation and boundary conditions for the viscous step.

We begin by considering a functional represented as

$$J[\phi] = \int_{\Omega} F(\mathbf{x}, \phi, \text{grad}\phi) dV. \quad (6.1.8)$$

The variation in this functional equals the difference between the functional evaluated at ϕ^* and ϕ . Thus, $\delta J = J[\phi^*] - J[\phi]$ may appear as

$$\delta J = \int_{\Omega} [F(\mathbf{x}, \phi + \epsilon\psi, \text{grad}\phi + \epsilon \text{grad}\psi) - F(\mathbf{x}, \phi, \text{grad}\phi)] dV. \quad (6.1.9)$$

Expanding the integrand in a Taylor series gives

$$\delta J = \int_{\Omega} \left[\frac{\partial F}{\partial \phi} \epsilon \cdot \psi + \frac{\partial F}{\partial \text{grad} \phi} \epsilon : \text{grad} \psi \right] dV, \quad (6.1.10)$$

which, after application of the chain rule, yields

$$\delta J = \epsilon \int_{\Omega} \left[\frac{\partial F}{\partial \phi} - \nabla \cdot \left(\frac{\partial F}{\partial \text{grad} \phi} \right) \right] \cdot \psi dV + \epsilon \int_{\Omega} \nabla \cdot \left(\frac{\partial F}{\partial \text{grad} \phi} \cdot \psi \right) dV. \quad (6.1.11)$$

Applying this expression to the functional in (6.1.7) results in

$$\begin{aligned} \delta J = \epsilon \int_{\Omega} [\nabla \cdot \text{grad} \phi - \lambda^2 \phi - F] \cdot \psi dV + \epsilon \int_{\Omega} \nabla \cdot [-\text{grad} \phi \cdot \psi] dV \\ + \epsilon \int_{\partial \Omega^n} \mathbf{g} \cdot \psi d\sigma. \end{aligned} \quad (6.1.12)$$

The divergence theorem allows us to express the second integral on the right as

$$\epsilon \int_{\Omega} \nabla \cdot [-\text{grad} \phi \cdot \psi] dV = -\epsilon \int_{\partial \Omega} \mathbf{n} \cdot (\text{grad} \phi \cdot \psi) d\sigma. \quad (6.1.13)$$

The integrand on the right-hand side equals zero along the boundary where essential conditions apply, since $\psi=0$ in those regions; the only contribution comes from boundaries containing natural boundary conditions. Using the natural boundary conditions given in (6.1.5) gives

$$\epsilon \int_{\Omega} \nabla \cdot [-\text{grad} \phi \cdot \psi] dV = -\epsilon \int_{\partial \Omega^n} \mathbf{g} \cdot \psi d\sigma \quad (6.1.14)$$

which exactly cancels the last term in (6.1.12). Thus, the variation in J equals

$$\delta J = \epsilon \int_{\Omega} [\nabla \cdot \text{grad} \phi - \lambda^2 \phi - F] \cdot \psi dV. \quad (6.1.15)$$

At an extremum, we require $\delta J=0$ for all admissible ψ ; in particular, we require $\delta J=0$ for all admissible ψ which vanish on the surface containing essential boundary conditions. Because of the arbitrariness of ψ inside Ω , $\delta J=0$ implies

$$\nabla^2 \phi - \lambda^2 \phi - F = 0, \text{ in } \Omega. \quad (6.1.16)$$

This equals Helmholtz's equation, confirming our supposition.

As indicated previously, the variational form incorporates the natural boundary conditions in the functional, while the essential boundary conditions do not appear. The functional expression makes no reference to a particular domain; hence, it applies to both a single element or the entire domain. In the following

sections we express this functional in terms of the local co-ordinates on a single element. Each element contributes both a volume integral and a corresponding surface integral. A functional applicable to the entire domain results from summing over all elements.

6.2 Representation in Local Co-Ordinates

The governing functional written in global, or physical space, equals

$$J[\phi] = \int_{\Omega} [-\frac{1}{2} \text{grad} \phi : \text{grad} \phi - \frac{1}{2} \lambda^2 \phi \cdot \phi - \phi \cdot F] dV + \int_{\partial \Omega^n} \phi \cdot g d\sigma. \quad (6.2.1)$$

We must transform the functional expression from the global (x,y,z) co-ordinate system to a local (r,s,t) system, where elements appear as cubes whose local co-ordinates range between ± 1 . The functional representation for a single element in local co-ordinates equals

$$J[\phi]^e = \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 [-\frac{1}{2} \text{grad} \phi : \text{grad} \phi - \frac{1}{2} \lambda^2 \phi \cdot \phi - \phi \cdot F]^e |\det[J^e]| dr ds dt + \sum_{p=1}^6 \int_{-1}^1 \int_{-1}^1 \phi^e \cdot g^e dA^p. \quad (6.2.2)$$

(Consult §A.3 for details of the differential volume conversion between global and local co-ordinates.) The surface integral expresses a summation over the six element faces. Remember, this term applies only along surfaces characterized by natural boundary conditions. Notice that the local co-ordinate system occupies a position within an element such that only two co-ordinates vary along a given face, while the third co-ordinate remains fixed at ± 1 . The gradient operator in the global system equals

$$\text{grad} \phi^e = \frac{\partial \phi^e}{\partial x} e_x + \frac{\partial \phi^e}{\partial y} e_y + \frac{\partial \phi^e}{\partial z} e_z. \quad (6.2.3)$$

In the local co-ordinate system, $[r(x,y,z), s(x,y,z), t(x,y,z)]$, this operator equals

$$\text{grad} \phi^e = [\frac{\partial \phi^e}{\partial r} r_x^e + \frac{\partial \phi^e}{\partial s} s_x^e + \frac{\partial \phi^e}{\partial t} t_x^e] e_x \quad (6.2.4)$$

$$+ [\frac{\partial \Phi^e}{\partial r} r_y^e + \frac{\partial \Phi^e}{\partial s} s_y^e + \frac{\partial \Phi^e}{\partial t} t_y^e] e_y + [\frac{\partial \Phi^e}{\partial r} r_z^e + \frac{\partial \Phi^e}{\partial s} s_z^e + \frac{\partial \Phi^e}{\partial t} t_z^e] e_z,$$

where the partial derivatives of the local co-ordinates with respect to the global ones appear according to (A.2.7) as

$$r_x^e = (\frac{y_s z_t - y_t z_s}{\det[J^e]})^e; \quad r_y^e = (\frac{x_t z_s - x_s z_t}{\det[J^e]})^e; \quad r_z^e = (\frac{x_s y_t - x_t y_s}{\det[J^e]})^e; \quad (6.2.5)$$

$$s_x^e = (\frac{y_t z_r - y_r z_t}{\det[J^e]})^e; \quad s_y^e = (\frac{x_r z_t - x_t z_r}{\det[J^e]})^e; \quad s_z^e = (\frac{x_t y_r - x_r y_t}{\det[J^e]})^e; \quad (6.2.6)$$

$$t_x^e = (\frac{y_r z_s - y_s z_r}{\det[J^e]})^e; \quad t_y^e = (\frac{x_s z_r - x_r z_s}{\det[J^e]})^e; \quad t_z^e = (\frac{x_r y_s - x_s y_r}{\det[J^e]})^e. \quad (6.2.7)$$

The Jacobian of the transformation equals

$$J^e = \begin{bmatrix} x_r & x_s & x_t \\ y_r & y_s & y_t \\ z_r & z_s & z_t \end{bmatrix}^e \quad (6.2.8)$$

according to §A.2. Subscripts indicate differentiation with respect to local co-ordinates; superscripts define the particular element under study.

6.3 Approximating Functions in Spectral Space

The discrete expansion of a function $u(r,s,t)$ in terms of a finite sequence of orthogonal functions of n -th degree approximately equals

$$u(r,s,t)^e \approx \sum_{i=0}^l \sum_{j=0}^m \sum_{k=0}^n \tilde{u}_{ijk}^e \psi_i(r) \psi_j(s) \psi_k(t), \quad (6.3.1)$$

where the scalars \tilde{u}_{ijk}^e equal the discrete expansion coefficients of $u(r,s,t)$ relative to the basis $\{\psi_0, \dots, \psi_n\}$. Notice that this expression is not of n -th degree unless $l=m=n$. As indicated in §1.5, differentiation may take place in either spectral space or physical space. Normally, we use differentiation in physical space. The derivative with respect to the local co-ordinate r in the local space equals

$$u_r(r,s,t)^e \approx \sum_{i=0}^l \sum_{j=0}^m \sum_{k=0}^n \tilde{u}_{ijk}^e \frac{\partial \psi_i(r)}{\partial r} \psi_j(s) \psi_k(t). \quad (6.3.2)$$

We do not compute derivatives in this manner since this would entail computing analytical expressions for the derivatives of the basis functions; instead, we compute derivatives only at the nodal points (r_a, s_b, t_c) . This gives

$$u_r(r_a, s_b, t_c)^e \approx \sum_{i=0}^1 \sum_{j=0}^m \sum_{k=0}^n \bar{u}_{ijk}^e \frac{\partial \psi_i(r_a)}{\partial r} \psi_j(s_b) \psi_k(t_c). \quad (6.3.3)$$

Since the basis functions satisfy both $\psi_i(r_a) = \delta_{ai}$ and $D_{ai} = \frac{\partial \psi_i}{\partial r}(r_a)$, this expression reduces to

$$u_r(r_a, s_b, t_c)^e \approx \sum_{i=0}^1 \sum_{j=0}^m \sum_{k=0}^n \bar{u}_{ijk}^e D_{ai} \delta_{bj} \delta_{ck}, \quad (6.3.4)$$

which may be written more compactly as

$$(u_r)_{abc}^e \approx \sum_{ijk} \bar{u}_{ijk}^e D_{ai} \delta_{bj} \delta_{ck}. \quad (6.3.5)$$

Similarly, derivatives with respect to the s and t directions equal

$$(u_s)_{abc}^e \approx \sum_{ijk} \bar{u}_{ijk}^e \delta_{ai} D_{bj} \delta_{ck} \quad (6.3.6)$$

and

$$(u_t)_{abc}^e \approx \sum_{ijk} \bar{u}_{ijk}^e \delta_{ai} \delta_{bj} D_{ck}, \quad (6.3.7)$$

respectively. The function $u(r, s, t)$ approximated at the node, (r_a, s_b, t_c) equals

$$u(r_a, s_b, t_c)^e \approx \sum_{i=0}^1 \sum_{j=0}^m \sum_{k=0}^n \bar{u}_{ijk}^e \psi_i(r_a) \psi_j(s_b) \psi_k(t_c) \quad (6.3.8)$$

or, in compact form,

$$u_{abc}^e \approx \sum_{ijk} \bar{u}_{ijk}^e \delta_{ai} \delta_{bj} \delta_{ck}. \quad (6.3.9)$$

With these expressions for functions and their derivatives, all the ingredients necessary to represent the functional in variational form exist. Incidentally, the first-order variational form, as opposed to the second-order differential form, does not require a second order derivative, clearly an advantage given the complexity of the first-order derivatives.

6.4 Approximation of Products of Functions

Since the variational form of our functional contains products of functions, some of which are known (e.g., the Jacobian or the body force), while others, such as velocity, remain unknown, we need a system to express products of functions. The two most common methods of expressing the product of functions u and v equal the product of the series,

$$u \cdot v \approx (I_n u)(I_n v), \quad (6.4.1)$$

or the series of the product,

$$u \cdot v \approx I_n(u \cdot v). \quad (6.4.2)$$

The first form yields a polynomial with n^2 terms since it involves term-by-term multiplication of two series; the second method involves a polynomial with n terms since the product u and v occurs before the expansion in terms of the nodal coefficients. We use the second method. Using the compact notation, the product of u and v equals

$$u^e \cdot v^e \approx \sum_{ijk} \bar{u}_{ijk}^e \cdot \bar{v}_{ijk}^e \psi_i(r) \psi_j(s) \psi_k(t). \quad (6.4.3)$$

A natural extension of this expression allows a representation of products of three or more terms.

6.5 Surface Integrals

The term representing the surface integral in (6.2.2) equals

$$I^e = \sum_{p=1}^6 I^{pe} = \sum_{p=1}^6 \int_{-1}^1 \int_{-1}^1 \phi^e \cdot \mathbf{g}^e dA^p. \quad (6.5.1)$$

Using the inhomogeneous boundary condition, $\mathbf{g} = (\mathbf{n} \cdot \nabla) \phi$, gives

$$I^e = \sum_{p=1}^6 \int_{-1}^1 \int_{-1}^1 \phi^e (\mathbf{n}^e \cdot \nabla) \phi^e dA^p, \quad (6.5.2)$$

which after rearranging gives

$$I^e = \sum_{p=1}^6 \int_{-1}^1 \int_{-1}^1 \phi^e (\mathbf{n}^e dA^p \cdot \nabla) \phi^e. \quad (6.5.3)$$

The projection of the differential surface area in the direction of the outward unit

normal on each of the six faces equals

$$\mathbf{n}^e dA^1 = - \begin{bmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ x_r & y_r & z_r \\ x_s & y_s & z_s \end{bmatrix}^e drds, \quad (6.5.4)$$

at $t=-1$;

$$\mathbf{n}^e dA^2 = \begin{bmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ x_r & y_r & z_r \\ x_t & y_t & z_t \end{bmatrix}^e drdt, \quad (6.5.5)$$

at $s=-1$;

$$\mathbf{n}^e dA^3 = \begin{bmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ x_r & y_r & z_r \\ x_s & y_s & z_s \end{bmatrix}^e drds, \quad (6.5.6)$$

at $t=1$;

$$\mathbf{n}^e dA^4 = - \begin{bmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ x_r & y_r & z_r \\ x_t & y_t & z_t \end{bmatrix}^e drdt, \quad (6.5.7)$$

at $s=1$;

$$\mathbf{n}^e dA^5 = - \begin{bmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ x_s & y_s & z_s \\ x_t & y_t & z_t \end{bmatrix}^e dsdt, \quad (6.5.8)$$

at $r=-1$; and

$$\mathbf{n}^e dA^6 = \begin{bmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ x_s & y_s & z_s \\ x_t & y_t & z_t \end{bmatrix}^e dsdt, \quad (6.5.9)$$

at $r=1$. (See §A.7 for details.) Taking the inner product of the projection of the differential area in the direction of the outward normal with the gradient operator for each of the six faces gives

$$\mathbf{n}^e dA^1 \cdot \nabla^e = - (t_x^e \frac{\partial}{\partial x} + t_y^e \frac{\partial}{\partial y} + t_z^e \frac{\partial}{\partial z}) \det[\mathbf{J}^e] drds, \quad (6.5.10)$$

on face 1;

$$\mathbf{n}^e dA^2 \cdot \nabla^e = - (s_x^e \frac{\partial}{\partial x} + s_y^e \frac{\partial}{\partial y} + s_z^e \frac{\partial}{\partial z}) \det[\mathbf{J}^e] drdt, \quad (6.5.11)$$

on face 2;

$$\mathbf{n}^e dA^3 \cdot \nabla^e = (t_x^e \frac{\partial}{\partial x} + t_y^e \frac{\partial}{\partial y} + t_z^e \frac{\partial}{\partial z}) \det[\mathbf{J}^e] drds, \quad (6.5.12)$$

on face 3;

$$\mathbf{n}^e dA^4 \cdot \nabla^e = (s_x^e \frac{\partial}{\partial x} + s_y^e \frac{\partial}{\partial y} + s_z^e \frac{\partial}{\partial z}) \det[\mathbf{J}^e] drdt, \quad (6.5.13)$$

on face 4;

$$\mathbf{n}^e dA^5 \cdot \nabla^e = - (r_x^e \frac{\partial}{\partial x} + r_y^e \frac{\partial}{\partial y} + r_z^e \frac{\partial}{\partial z}) \det[\mathbf{J}^e] ds dt, \quad (6.5.14)$$

on face 5; and

$$\mathbf{n}^e dA^6 \cdot \nabla^e = (r_x^e \frac{\partial}{\partial x} + r_y^e \frac{\partial}{\partial y} + r_z^e \frac{\partial}{\partial z}) \det[\mathbf{J}^e] ds dt, \quad (6.5.15)$$

on face 6, where the derivation of such quantities as $t_x = \partial t / \partial x$ appear in §A.2.

Substituting these expressions into (6.5.3) gives for each of the six faces:

$$I^{1e} = - \int_{-1}^1 \int_{-1}^1 \phi^e (t_x^e \frac{\partial \phi^e}{\partial x} + t_y^e \frac{\partial \phi^e}{\partial y} + t_z^e \frac{\partial \phi^e}{\partial z}) \det[\mathbf{J}^e] dr ds, \quad (6.5.16)$$

on face 1;

$$I^{2e} = - \int_{-1}^1 \int_{-1}^1 \phi^e (s_x^e \frac{\partial \phi^e}{\partial x} + s_y^e \frac{\partial \phi^e}{\partial y} + s_z^e \frac{\partial \phi^e}{\partial z}) \det[\mathbf{J}^e] dr dt, \quad (6.5.17)$$

on face 2;

$$I^{3e} = \int_{-1}^1 \int_{-1}^1 \phi^e (t_x^e \frac{\partial \phi^e}{\partial x} + t_y^e \frac{\partial \phi^e}{\partial y} + t_z^e \frac{\partial \phi^e}{\partial z}) \det[\mathbf{J}^e] dr ds, \quad (6.5.18)$$

on face 3;

$$I^{4e} = \int_{-1}^1 \int_{-1}^1 \phi^e (s_x^e \frac{\partial \phi^e}{\partial x} + s_y^e \frac{\partial \phi^e}{\partial y} + s_z^e \frac{\partial \phi^e}{\partial z}) \det[\mathbf{J}^e] dr dt, \quad (6.5.19)$$

on face 4;

$$I^{5e} = - \int_{-1}^1 \int_{-1}^1 \phi^e (r_x^e \frac{\partial \phi^e}{\partial x} + r_y^e \frac{\partial \phi^e}{\partial y} + r_z^e \frac{\partial \phi^e}{\partial z}) \det[\mathbf{J}^e] ds dt, \quad (6.5.20)$$

on face 5; and

$$I^{6e} = \int_{-1}^1 \int_{-1}^1 \phi^e (r_x^e \frac{\partial \phi^e}{\partial x} + r_y^e \frac{\partial \phi^e}{\partial y} + r_z^e \frac{\partial \phi^e}{\partial z}) \det[\mathbf{J}^e] ds dt, \quad (6.5.21)$$

on face 6.

Substituting the expression for the derivatives $\frac{\partial \phi^e}{\partial x}$, $\frac{\partial \phi^e}{\partial y}$, and $\frac{\partial \phi^e}{\partial z}$ from (6.2.4) into the surface integral for face 1, gives

$$\begin{aligned} I^{1e} = - \int_{-1}^1 \int_{-1}^1 [& t_x^e (r_x^e \frac{\partial \phi^e}{\partial r} + s_x^e \frac{\partial \phi^e}{\partial s} + t_x^e \frac{\partial \phi^e}{\partial t}) + t_y^e (r_y^e \frac{\partial \phi^e}{\partial r} + s_y^e \frac{\partial \phi^e}{\partial s} + t_y^e \frac{\partial \phi^e}{\partial t}) \\ & + t_z^e (r_z^e \frac{\partial \phi^e}{\partial r} + s_z^e \frac{\partial \phi^e}{\partial s} + t_z^e \frac{\partial \phi^e}{\partial t})] \phi^e \det[\mathbf{J}^e] dr ds. \end{aligned} \quad (6.5.22)$$

We must introduce the expansion polynomials and coefficients into these integral

expressions. The result for face 1 equals

$$I^{1e} \approx - \int_{-1}^1 \int_{-1}^1 \sum_{ab} [t_x^e(r_x^e \frac{\partial \phi^e}{\partial r} + s_x^e \frac{\partial \phi^e}{\partial s} + t_z^e \frac{\partial \phi^e}{\partial t}) + t_y^e(r_y^e \frac{\partial \phi^e}{\partial r} + s_y^e \frac{\partial \phi^e}{\partial s} + t_y^e \frac{\partial \phi^e}{\partial t}) + t_z^e(r_z^e \frac{\partial \phi^e}{\partial r} + s_z^e \frac{\partial \phi^e}{\partial s} + t_z^e \frac{\partial \phi^e}{\partial t})]_{ab} \det[J^e]_{ab} \phi_{ab}^e \psi_a(r) \psi_b(s) dr ds, \quad (6.5.23)$$

assuming the quantity within square brackets refers to the nodal points at r_a, s_b, t_1 . Similar expressions apply for faces 2 through 6. Substituting expressions for the partial derivatives of ϕ from (6.3.5), (6.3.6), and (6.3.7) gives

$$I^{1e} \approx - \int_{-1}^1 \int_{-1}^1 \sum_{ab} \sum_{ijk} [t_x^e(r_x^e D_{ai} \delta_{bj} \delta_{1k} + s_x^e \delta_{ai} D_{bj} \delta_{1k} + t_x^e \delta_{ai} \delta_{bj} D_{1k}) + t_y(r_y^e D_{ai} \delta_{bj} \delta_{1k} + s_y^e \delta_{ai} D_{bj} \delta_{1k} + t_y^e \delta_{ai} \delta_{bj} D_{1k}) + t_z^e(r_z^e D_{ai} \delta_{bj} \delta_{1k} + s_z^e \delta_{ai} D_{bj} \delta_{1k} + t_z^e \delta_{ai} \delta_{bj} D_{1k})]_{ab} \tilde{\phi}_{ijk}^e \tilde{\phi}_{ab}^e \det[J^e]_{ab} \psi_a(r) \psi_b(s) dr ds. \quad (6.5.24)$$

The only variables remaining within the integrand equal $\psi(r)$, $\psi(s)$, and $\psi(t)$; therefore, integration reduces to $\int_{-1}^1 \psi_i(r) dr = w_i$. Substituting these expressions into (6.5.24) gives

$$I^{1e} \approx - \sum_{ab} \sum_{ijk} [t_x^e(r_x^e D_{ai} \delta_{bj} \delta_{1k} + s_x^e \delta_{ai} D_{bj} \delta_{1k} + t_x^e \delta_{ai} \delta_{bj} D_{1k}) + t_y(r_y^e D_{ai} \delta_{bj} \delta_{1k} + s_y^e \delta_{ai} D_{bj} \delta_{1k} + t_y^e \delta_{ai} \delta_{bj} D_{1k}) + t_z^e(r_z^e D_{ai} \delta_{bj} \delta_{1k} + s_z^e \delta_{ai} D_{bj} \delta_{1k} + t_z^e \delta_{ai} \delta_{bj} D_{1k})]_{ab} \tilde{\phi}_{ijk}^e \tilde{\phi}_{ab}^e \det[J^e]_{ab} w_a w_b. \quad (6.5.25)$$

The superscript tilde identifies unknown discrete expansion coefficients. The other terms do not contain the tilde (e.g., t_x^e, r_x^e and $\det[J^e]$) since they represent known continuous functions which do not require expression in terms of approximate expansion coefficients—these coefficients depend on evaluation of functions at the nodes. For completeness, the surface integrals for faces 2 through 6 equal

$$I^{2e} \approx - \sum_{ac} \sum_{ijk} [s_x^e(r_x^e D_{ai} \delta_{2j} \delta_{ck} + s_x^e \delta_{ai} D_{2j} \delta_{ck} + t_x^e \delta_{ai} \delta_{2j} D_{ck}) + s_y(r_y^e D_{ai} \delta_{2j} \delta_{ck} + s_y^e \delta_{ai} D_{2j} \delta_{ck} + t_y^e \delta_{ai} \delta_{2j} D_{ck}) + s_z^e(r_z^e D_{ai} \delta_{2j} \delta_{ck} + s_z^e \delta_{ai} D_{2j} \delta_{ck} + t_z^e \delta_{ai} \delta_{2j} D_{ck}) + \dots]_{ac} \tilde{\phi}_{ijk}^e \tilde{\phi}_{ac}^e \det[J^e]_{ac} w_a w_c. \quad (6.5.26)$$

$$s_z^e \delta_{ai} D_{2j} \delta_{ck} + t_z^e \delta_{ai} \delta_{2j} D_{ck})]_{ab} \Phi_{ijk}^e \Phi_{a2c}^e \det[J^e]_{a2c} w_a w_c; \quad (6.5.27)$$

$$I^{3e} \approx$$

$$\sum_{ab} \sum_{ijk} [t_x^e (r_x^e D_{ai} \delta_{bj} \delta_{2k} + s_x^e \delta_{ai} D_{bj} \delta_{2k} + t_x^e \delta_{ai} \delta_{bj} D_{2k}) + t_y (r_y^e D_{ai} \delta_{bj} \delta_{2k} + s_y^e \delta_{ai} D_{bj} \delta_{2k} + t_y^e \delta_{ai} \delta_{bj} D_{2k}) + t_z^e (r_z^e D_{ai} \delta_{bj} \delta_{2k} + s_z^e \delta_{ai} D_{bj} \delta_{2k} + t_z^e \delta_{ai} \delta_{bj} D_{2k})]_{ab} \Phi_{ijk}^e \Phi_{ab2}^e \det[J^e]_{ab2} w_a w_b; \quad (6.5.28)$$

$$I^{4e} \approx$$

$$\sum_{ac} \sum_{ijk} [s_x^e (r_x^e D_{ai} \delta_{1j} \delta_{ck} + s_x^e \delta_{ai} D_{1j} \delta_{ck} + t_x^e \delta_{ai} \delta_{1j} D_{ck}) + s_y (r_y^e D_{ai} \delta_{1j} \delta_{ck} + s_y^e \delta_{ai} D_{1j} \delta_{ck} + t_y^e \delta_{ai} \delta_{1j} D_{ck}) + s_z^e (r_z^e D_{ai} \delta_{1j} \delta_{ck} + s_z^e \delta_{ai} D_{1j} \delta_{ck} + t_z^e \delta_{ai} \delta_{1j} D_{ck})]_{ab} \Phi_{ijk}^e \Phi_{a1c}^e \det[J^e]_{a1c} w_a w_c; \quad (6.5.29)$$

$$I^{5e} \approx$$

$$- \sum_{bc} \sum_{ijk} [r_x^e (r_x^e D_{1i} \delta_{bj} \delta_{ck} + s_x^e \delta_{1i} D_{bj} \delta_{ck} + t_x^e \delta_{1i} \delta_{bj} D_{ck}) + r_y (r_y^e D_{1i} \delta_{bj} \delta_{ck} + s_y^e \delta_{1i} D_{bj} \delta_{ck} + t_y^e \delta_{1i} \delta_{bj} D_{ck}) + r_z^e (r_z^e D_{1i} \delta_{bj} \delta_{ck} + s_z^e \delta_{1i} D_{bj} \delta_{ck} + t_z^e \delta_{1i} \delta_{bj} D_{ck})]_{1bc} \Phi_{ijk}^e \Phi_{1bc}^e \det[J^e]_{1bc} w_b w_c; \text{ and} \quad (6.5.30)$$

$$I^{6e} \approx$$

$$\sum_{bc} \sum_{ijk} [r_x^e (r_x^e D_{2i} \delta_{bj} \delta_{ck} + s_x^e \delta_{2i} D_{bj} \delta_{ck} + t_x^e \delta_{2i} \delta_{bj} D_{ck}) + r_y (r_y^e D_{2i} \delta_{bj} \delta_{ck} + s_y^e \delta_{2i} D_{bj} \delta_{ck} + t_y^e \delta_{2i} \delta_{bj} D_{ck}) + r_z^e (r_z^e D_{2i} \delta_{bj} \delta_{ck} + s_z^e \delta_{2i} D_{bj} \delta_{ck} + t_z^e \delta_{2i} \delta_{bj} D_{ck})]_{2bc} \Phi_{ijk}^e \Phi_{2bc}^e \det[J^e]_{2bc} w_b w_c.$$

6.6 Application to Variational Form

The governing functional approximated in discrete form equals

$$J[\Phi]^e \approx \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \sum_{-1abc} [-\frac{1}{2} \nabla_{abc}^e \Phi_{abc}^e : \nabla_{abc}^e \Phi_{abc}^e - \frac{1}{2} \lambda^2 \Phi_{abc}^e \cdot \Phi_{abc}^e - \Phi_{abc}^e \cdot F_{abc}] \psi_a(r) \psi_b(s) \psi_c(t) |\det[J^e]|_{abc} dr ds dt + \sum_{p=1}^6 I^{pe}. \quad (6.6.1)$$

The first term within the integral on the right-hand side appears as

$$\nabla_{abc}^e \Phi_{abc}^e : \nabla_{abc}^e \Phi_{abc}^e = \left[\left(\frac{\partial \Phi^e}{\partial r} \right)_{abc} (r_x)_{abc}^e + \left(\frac{\partial \Phi^e}{\partial s} \right)_{abc} (s_x)_{abc}^e + \left(\frac{\partial \Phi^e}{\partial t} \right)_{abc} (t_x)_{abc}^e \right] e_x \quad (6.6.2)$$

$$\begin{aligned}
& [(\frac{\partial \Phi^e}{\partial r})_{abc}(r_y)_{abc}^e + (\frac{\partial \Phi^e}{\partial s})_{abc}(s_y)_{abc}^e + (\frac{\partial \Phi^e}{\partial t})_{abc}(t_y)_{abc}^e]e_y \\
& [(\frac{\partial \Phi^e}{\partial r})_{abc}(r_z)_{abc}^e + (\frac{\partial \Phi^e}{\partial s})_{abc}(s_z)_{abc}^e + (\frac{\partial \Phi^e}{\partial t})_{abc}(t_z)_{abc}^e]e_z \Big] \cdot \\
& \Big[[(\frac{\partial \Phi^e}{\partial r})_{abc}(r_x)_{abc}^e + (\frac{\partial \Phi^e}{\partial s})_{abc}(s_x)_{abc}^e + (\frac{\partial \Phi^e}{\partial t})_{abc}(t_x)_{abc}^e]e_x \\
& [(\frac{\partial \Phi^e}{\partial r})_{abc}(r_y)_{abc}^e + (\frac{\partial \Phi^e}{\partial s})_{abc}(s_y)_{abc}^e + (\frac{\partial \Phi^e}{\partial t})_{abc}(t_y)_{abc}^e]e_y \\
& [(\frac{\partial \Phi^e}{\partial r})_{abc}(r_z)_{abc}^e + (\frac{\partial \Phi^e}{\partial s})_{abc}(s_z)_{abc}^e + (\frac{\partial \Phi^e}{\partial t})_{abc}(t_z)_{abc}^e]e_z \Big].
\end{aligned}$$

Performing the inner product and introducing the discrete expansions for the partial derivatives gives

$$\begin{aligned}
\nabla_{abc}^e \Phi_{abc}^e : \nabla_{abc}^e \Phi_{abc}^e &= \sum_{ijk} \sum_{lmn} \Phi_{ijk}^e \cdot \Phi_{lmn}^e \quad (6.6.3) \\
& \Big[[(r_x)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (s_x)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (t_x)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_x)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (s_x)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (t_x)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_y)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (s_y)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (t_y)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_y)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (s_y)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (t_y)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_z)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (s_z)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (t_z)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_z)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (s_z)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (t_z)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] \Big].
\end{aligned}$$

Substituting this relation into (6.6.1) gives

$$\begin{aligned}
J[\Phi]^e &\approx \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \sum_{abc} \psi_a(r) \psi_b(s) \psi_c(t) |\det[J^e]|_{abc} \Big[-\frac{1}{2} \sum_{ijk} \sum_{lmn} \Phi_{ijk}^e \cdot \Phi_{lmn}^e \\
& \Big[[(r_x)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (s_x)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (t_x)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_x)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (s_x)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (t_x)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_y)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (s_y)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (t_y)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_y)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (s_y)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (t_y)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] + \\
& [(r_z)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (s_z)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (t_z)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \\
& [(r_z)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (s_z)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (t_z)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] \Big] \\
& - \frac{1}{2} \lambda^2 \Phi_{abc}^e \cdot \Phi_{abc}^e - \Phi_{abc}^e \cdot F_{abc}^e \Big] dr ds dt + \sum_{p=1}^6 I P^e. \quad (6.6.4)
\end{aligned}$$

Again, the only variables within the integrand equal $\psi(r)$, $\psi(s)$, and $\psi(t)$.

Using (1.5.16) for $\int_{-1}^1 \psi_i(x) dx$ gives

$$\begin{aligned}
J[\phi]^e &\approx -\frac{1}{4} \sum_{abc} \sum_{ijk} \sum_{lmn} \phi_{ijk}^e \cdot \phi_{lmn}^e |\det[J^e]|_{abc} w_a w_b w_c \\
&\left[[(I_x)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (S_x)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (T_x)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \right. \\
&[(I_x)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (S_x)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (T_x)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] + \\
&[(I_y)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (S_y)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (T_y)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \\
&[(I_y)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (S_y)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (T_y)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] + \\
&[(I_z)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (S_z)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (T_z)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \\
&\left. [(I_z)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (S_z)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (T_z)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] \right] \\
&- \frac{1}{4} \lambda^2 \sum_{lmn} \phi_{lmn}^e \cdot \phi_{lmn}^e |\det[J^e]|_{lmn} w_l w_m w_n \\
&- \sum_{lmn} \phi_{lmn}^e \cdot F_{lmn}^e |\det[J^e]|_{lmn} w_l w_m w_n + \sum_{p=1}^6 I^{pe}. \quad (6.6.5)
\end{aligned}$$

The equation which minimizes the functional $J[\phi]$ occurs when $\delta J / \delta \phi_{lmn} = 0$, and equals

$$\begin{aligned}
\frac{\partial J^e}{\partial \phi_{lmn}} &\approx - \sum_{abc} \sum_{ijk} \phi_{ijk}^e |\det[J^e]|_{abc} w_a w_b w_c \quad (6.6.6) \\
&\left[[(I_x)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (S_x)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (T_x)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \right. \\
&[(I_x)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (S_x)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (T_x)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] + \\
&[(I_y)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (S_y)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (T_y)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \\
&[(I_y)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (S_y)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (T_y)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] + \\
&[(I_z)_{abc}^e D_{ai} \delta_{bj} \delta_{ck} + (S_z)_{abc}^e \delta_{ai} D_{bj} \delta_{ck} + (T_z)_{abc}^e \delta_{ai} \delta_{bj} D_{ck}] \\
&\left. [(I_z)_{abc}^e D_{al} \delta_{bm} \delta_{cn} + (S_z)_{abc}^e \delta_{al} D_{bm} \delta_{cn} + (T_z)_{abc}^e \delta_{al} \delta_{bm} D_{cn}] \right] \\
&- \lambda^2 \phi_{lmn}^e |\det[J^e]|_{lmn} w_l w_m w_n - F_{lmn}^e |\det[J^e]|_{lmn} w_l w_m w_n + \\
&\iint_{\partial \Omega} \mathbf{n} \cdot \frac{\partial F}{\partial \text{grad} \phi} d\sigma + \frac{\partial}{\partial \phi} \left[\sum_{p=1}^6 I^{pe} \right].
\end{aligned}$$

The last two terms cancel.† Setting $\delta J / \delta \phi_{lmn} = 0$ gives a more compact form of

†The integrand of the second-last term equals $\mathbf{n} \cdot \partial F / \partial \text{grad} \phi$ which also equals $-\mathbf{n} \cdot \text{grad} \phi$ for the functional defined in (6.2.2). The integration of this term takes place over both the essential and natural boundaries. The variation of the surface integral with respect to ϕ equals g integrated over the boundary where

(6.6.6):

$$\sum_{ijk} [\Lambda_{lmnijk}^e - \lambda^2 \Pi_{lmnijk}^e] \phi_{ijk}^e = \sum_{ijk} \Pi_{lmnijk}^e F_{ijk}^e, \quad (6.6.7)$$

where Π and Λ appear as

$$\Pi_{lmnijk}^e \equiv -|\det[J^e]|_{ijk} w_i w_j w_k \delta_{li} \delta_{mj} \delta_{nk} \quad (6.6.8)$$

and

$$\begin{aligned} \Lambda_{lmnijk}^e \equiv \sum_{abc} |\det[J^e]|_{abc} w_a w_b w_c [& \\ & [(r_x)^e_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_x)^e_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_x)^e_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\ & [(r_x)^e_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_x)^e_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_x)^e_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\ & [(r_y)^e_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_y)^e_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_y)^e_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\ & [(r_y)^e_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_y)^e_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_y)^e_{abc} \delta_{al} \delta_{bm} D_{cn}] + \\ & [(r_z)^e_{abc} D_{ai} \delta_{bj} \delta_{ck} + (s_z)^e_{abc} \delta_{ai} D_{bj} \delta_{ck} + (t_z)^e_{abc} \delta_{ai} \delta_{bj} D_{ck}] \\ & [(r_z)^e_{abc} D_{al} \delta_{bm} \delta_{cn} + (s_z)^e_{abc} \delta_{al} D_{bm} \delta_{cn} + (t_z)^e_{abc} \delta_{al} \delta_{bm} D_{cn}]]. \end{aligned} \quad (6.6.9)$$

Performing the multiplication associated with (6.6.9) gives

$$\begin{aligned} \Lambda_{lmnijk}^e = \sum_{abc} \det[J^e]_{abc} w_a w_b w_c [& \\ & (r_x^e r_x^e + r_y^e r_y^e + r_z^e r_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} D_{al} \delta_{bm} \delta_{cn} + \\ & (r_x^e s_x^e + r_y^e s_y^e + r_z^e s_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} \delta_{al} D_{bm} \delta_{cn} + \\ & (r_x^e t_x^e + r_y^e t_y^e + r_z^e t_z^e)_{abc} D_{ai} \delta_{bj} \delta_{ck} \delta_{al} \delta_{bm} D_{cn} + \\ & (s_x^e r_x^e + s_y^e r_y^e + s_z^e r_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} D_{al} \delta_{bm} \delta_{cn} + \\ & (s_x^e s_x^e + s_y^e s_y^e + s_z^e s_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} \delta_{al} D_{bm} \delta_{cn} + \\ & (s_x^e t_x^e + s_y^e t_y^e + s_z^e t_z^e)_{abc} \delta_{ai} D_{bj} \delta_{ck} \delta_{al} \delta_{bm} D_{cn} + \\ & (t_x^e r_x^e + t_y^e r_y^e + t_z^e r_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck} D_{al} \delta_{bm} \delta_{cn} + \\ & (t_x^e s_x^e + t_y^e s_y^e + t_z^e s_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck} \delta_{al} D_{bm} \delta_{cn} + \\ & (t_x^e t_x^e + t_y^e t_y^e + t_z^e t_z^e)_{abc} \delta_{ai} \delta_{bj} D_{ck} \delta_{al} \delta_{bm} D_{cn}]. \end{aligned} \quad (6.6.10)$$

natural conditions exist. Since g equals $n\text{-grad}\phi$, these terms cancel along the boundary where the natural conditions apply; the variation of ϕ along the boundaries where essential boundary conditions apply equals zero. Whence, these terms contribute nothing to the variation of $J[\phi]$.

This expression simplifies after contracting on the free indices associated with the Kronecker delta; this requires several steps. First, multiply (6.6.10) by ϕ_{ijk} and contract on the indices a , b , and c giving

$$\begin{aligned} \sum_{ijk} \Lambda_{lmnijk}^e \phi_{ijk}^e = & \quad (6.6.11) \\ & \sum_{ijk} \sum_a (r_x^e r_x^e + r_y^e r_y^e + r_z^e r_z^e)_{amn} D_{ai} \delta_{mj} \delta_{nk} D_{al} |\det[J^e]|_{amn} w_a w_m w_n \phi_{ijk}^e \\ & + \sum_{ijk} \sum_b (r_x^e s_x^e + r_y^e s_y^e + r_z^e s_z^e)_{lbn} D_{li} \delta_{bj} \delta_{nk} D_{bm} |\det[J^e]|_{lbn} w_l w_b w_n \phi_{ijk}^e \\ & + \sum_{ijk} \sum_c (r_x^e t_x^e + r_y^e t_y^e + r_z^e t_z^e)_{lmc} D_{li} \delta_{mj} \delta_{ck} D_{cn} |\det[J^e]|_{lmc} w_l w_m w_c \phi_{ijk}^e \\ & + \sum_{ijk} \sum_a (s_x^e r_x^e + s_y^e r_y^e + s_z^e r_z^e)_{amn} \delta_{ai} D_{mj} \delta_{nk} D_{al} |\det[J^e]|_{amn} w_a w_m w_n \phi_{ijk}^e \\ & + \sum_{ijk} \sum_b (s_x^e s_x^e + s_y^e s_y^e + s_z^e s_z^e)_{lbn} \delta_{li} D_{bj} \delta_{nk} D_{bm} |\det[J^e]|_{lbn} w_l w_b w_n \phi_{ijk}^e \\ & + \sum_{ijk} \sum_c (s_x^e t_x^e + s_y^e t_y^e + s_z^e t_z^e)_{lmc} \delta_{li} D_{mj} \delta_{ck} D_{cn} |\det[J^e]|_{lmc} w_l w_m w_c \phi_{ijk}^e \\ & + \sum_{ijk} \sum_a (t_x^e r_x^e + t_y^e r_y^e + t_z^e r_z^e)_{amn} \delta_{ai} \delta_{mj} D_{nk} D_{al} |\det[J^e]|_{amn} w_a w_m w_n \phi_{ijk}^e \\ & + \sum_{ijk} \sum_b (t_x^e s_x^e + t_y^e s_y^e + t_z^e s_z^e)_{lbn} \delta_{li} \delta_{bj} D_{nk} D_{bm} |\det[J^e]|_{lbn} w_l w_b w_n \phi_{ijk}^e \\ & + \sum_{ijk} \sum_c (t_x^e t_x^e + t_y^e t_y^e + t_z^e t_z^e)_{lmc} \delta_{li} \delta_{mj} D_{ck} D_{cn} |\det[J^e]|_{lmc} w_l w_m w_c \phi_{ijk}^e. \end{aligned}$$

Using the properties of the Kronecker delta while contracting on the indices i , j and k gives

$$\begin{aligned} \sum_{ijk} \Lambda_{lmnijk}^e \phi_{ijk}^e = & \quad (6.6.12) \\ & \sum_{ia} (r_x^e r_x^e + r_y^e r_y^e + r_z^e r_z^e)_{amn} D_{ai}^l D_{al}^l |\det[J^e]|_{amn} w_a w_m w_n \phi_{imn}^e \\ & + \sum_{ib} (r_x^e s_x^e + r_y^e s_y^e + r_z^e s_z^e)_{lbn} D_{li}^l D_{bm}^l |\det[J^e]|_{lbn} w_l w_b w_n \phi_{ibn}^e \\ & + \sum_{ic} (r_x^e t_x^e + r_y^e t_y^e + r_z^e t_z^e)_{lmc} D_{li}^l D_{cn}^l |\det[J^e]|_{lmc} w_l w_m w_c \phi_{imc}^e \\ & + \sum_{ja} (s_x^e r_x^e + s_y^e r_y^e + s_z^e r_z^e)_{amn} D_{mj}^l D_{al}^l |\det[J^e]|_{amn} w_a w_m w_n \phi_{ajn}^e \\ & + \sum_{jb} (s_x^e s_x^e + s_y^e s_y^e + s_z^e s_z^e)_{lbn} D_{bj}^l D_{bm}^l |\det[J^e]|_{lbn} w_l w_b w_n \phi_{lbn}^e \\ & + \sum_{jc} (s_x^e t_x^e + s_y^e t_y^e + s_z^e t_z^e)_{lmc} D_{mj}^l D_{cn}^l |\det[J^e]|_{lmc} w_l w_m w_c \phi_{lmc}^e \\ & + \sum_{ka} (t_x^e r_x^e + t_y^e r_y^e + t_z^e r_z^e)_{amn} D_{nk}^l D_{al}^l |\det[J^e]|_{amn} w_a w_m w_n \phi_{amk}^e \\ & + \sum_{kb} (t_x^e s_x^e + t_y^e s_y^e + t_z^e s_z^e)_{lbn} D_{nk}^l D_{bm}^l |\det[J^e]|_{lbn} w_l w_b w_n \phi_{lbn}^e \\ & + \sum_{kc} (t_x^e t_x^e + t_y^e t_y^e + t_z^e t_z^e)_{lmc} D_{ck}^l D_{cn}^l |\det[J^e]|_{lmc} w_l w_m w_c \phi_{emk}^e. \end{aligned}$$

The superscripts on D indicate the local direction associated with the derivative. We must maintain this designation, since, in general, the number of nodes in each of the three local directions differ. In other words, the quantities D^r , D^s , and D^t differ. A simplification occurs upon introduction of the symmetric array of coefficients,

$$(C_{11})_{amn}^e \equiv \quad (6.6.13)$$

$$(r_x^e r_x^e + r_y^e r_y^e + r_z^e r_z^e)_{amn} |\det[J^e]|_{amn} w_a w_m w_n,$$

$$(C_{12})_{lbn} \equiv \quad (6.6.14)$$

$$(r_x^e s_x^e + r_y^e s_y^e + r_z^e s_z^e)_{lbn} |\det[J^e]|_{lbn} w_l w_b w_n,$$

$$(C_{13})_{lmc} \equiv \quad (6.6.15)$$

$$(r_x^e t_x^e + r_y^e t_y^e + r_z^e t_z^e)_{lmc} |\det[J^e]|_{lmc} w_l w_m w_c,$$

$$(C_{21})_{amn}^e \equiv \quad (6.6.16)$$

$$(s_x^e r_x^e + s_y^e r_y^e + s_z^e r_z^e)_{amn} |\det[J^e]|_{amn} w_a w_m w_n,$$

$$(C_{22})_{lbn} \equiv \quad (6.6.17)$$

$$(s_x^e s_x^e + s_y^e s_y^e + s_z^e s_z^e)_{lbn} |\det[J^e]|_{lbn} w_l w_b w_n,$$

$$(C_{23})_{lmc} \equiv \quad (6.6.18)$$

$$(s_x^e t_x^e + s_y^e t_y^e + s_z^e t_z^e)_{lmc} |\det[J^e]|_{lmc} w_l w_m w_c,$$

$$(C_{31})_{amn}^e \equiv \quad (6.6.19)$$

$$(t_x^e r_x^e + t_y^e r_y^e + t_z^e r_z^e)_{amn} |\det[J^e]|_{amn} w_a w_m w_n,$$

$$(C_{32})_{lbn} \equiv \quad (6.6.20)$$

$$(t_x^e s_x^e + t_y^e s_y^e + t_z^e s_z^e)_{lbn} |\det[J^e]|_{lbn} w_l w_b w_n,$$

$$\text{and} \quad (C_{33})_{lmc} \equiv \quad (6.6.21)$$

$$(t_x^e t_x^e + t_y^e t_y^e + t_z^e t_z^e)_{lmc} |\det[J^e]|_{lmc} w_l w_m w_c,$$

into (6.6.12), giving

$$\sum_{ijk} \Lambda_{lmnijk}^e \phi_{ijk}^e = \quad (6.6.22)$$

$$\begin{aligned}
& \sum_{ia} (C_{11})_{amn}^e D_{ai}^r D_{al}^r \phi_{imn}^e + \sum_{ib} (C_{12})_{bmn}^e D_{bi}^r D_{bm}^s \phi_{ibn}^e + \\
& \sum_{ic} (C_{13})_{imc}^e D_{ci}^r D_{cn}^t \phi_{imc}^e + \sum_{ja} (C_{12})_{amn}^e D_{mj}^s D_{al}^r \phi_{ajn}^e + \\
& \sum_{jb} (C_{22})_{bmn}^e D_{bj}^s D_{bm}^s \phi_{ijb}^e + \sum_{jc} (C_{23})_{imc}^e D_{mj}^s D_{cn}^t \phi_{ijc}^e + \\
& \sum_{ka} (C_{13})_{amn}^e D_{nk}^t D_{al}^r \phi_{amk}^e + \sum_{kb} (C_{23})_{bmn}^e D_{nk}^t D_{bm}^s \phi_{ibk}^e + \\
& \sum_{kc} (C_{33})_{imc}^e D_{ck}^t D_{cn}^t \phi_{imk}^e.
\end{aligned}$$

Reordering the terms in this relation yields

$$\begin{aligned}
& \sum_{ijk} \Lambda_{imnij}^e \phi_{ijk}^e = \quad (6.6.23) \\
& \sum_{ia} (C_{11})_{amn}^e D_{ai}^r D_{al}^r \phi_{imn}^e + \sum_{ja} (C_{12})_{amn}^e D_{aj}^s D_{al}^r \phi_{ajn}^e + \\
& \sum_{ka} (C_{13})_{amn}^e D_{al}^r D_{nk}^t \phi_{amk}^e + \sum_{ib} (C_{12})_{bmn}^e D_{bi}^r D_{bm}^s \phi_{ibn}^e + \\
& \sum_{jb} (C_{22})_{bmn}^e D_{bj}^s D_{bm}^s \phi_{ijb}^e + \sum_{kb} (C_{23})_{bmn}^e D_{bm}^s D_{nk}^t \phi_{ibk}^e + \\
& \sum_{ic} (C_{13})_{imc}^e D_{cn}^t D_{ci}^r \phi_{imc}^e + \sum_{jc} (C_{23})_{imc}^e D_{cn}^t D_{mj}^s \phi_{ijc}^e + \sum_{kc} (C_{33})_{imc}^e D_{ck}^t D_{cn}^t \phi_{imk}^e.
\end{aligned}$$

Further arrangements produce

$$\begin{aligned}
& \sum_{ijk} \Lambda_{imnij}^e \phi_{ijk}^e = \quad (6.6.24) \\
& \sum_a (D_{la}^t)^\dagger \left[\sum_i (C_{11})_{amn}^e (D_{ai}^r \phi_{imn}^e) + \sum_j (C_{12})_{amn}^e (D_{mj}^s \phi_{ajn}^e) + \sum_k (C_{13})_{amn}^e (D_{nk}^t \phi_{amk}^e) \right] + \\
& \sum_b \left[\sum_i (C_{12})_{bmn}^e (D_{bi}^r \phi_{ibn}^e) + \sum_j (C_{22})_{bmn}^e (D_{bj}^s \phi_{ijb}^e) + \sum_k (C_{23})_{bmn}^e (D_{nk}^t \phi_{ibk}^e) \right] D_{bm}^s + \\
& \sum_c \left[\sum_i (C_{13})_{imc}^e (D_{ci}^r \phi_{imc}^e) + \sum_j (C_{23})_{imc}^e (D_{mj}^s \phi_{ijc}^e) + \sum_k (C_{33})_{imc}^e (D_{ck}^t \phi_{imk}^e) \right] D_{cn}^t.^\dagger
\end{aligned}$$

Introducing

$$B_{amn}^r \equiv \sum_i D_{ai}^r \phi_{imn}^e, \quad (6.6.25)$$

$$B_{amn}^s \equiv \sum_j D_{mj}^s \phi_{ajn}^e, \quad (6.6.26)$$

and

$$B_{amn}^t \equiv \sum_k D_{nk}^t \phi_{amk}^e, \quad (6.6.27)$$

and substituting into (6.6.24) gives

†The quantities within parentheses, for example $D_{ai} \phi_{imn}^e$, can be written as A_{am} after performing the matrix multiplication. In this form the product $D_{al} A_{am}$ does not satisfy the rules of matrix multiplication. In matrix multiplication the second index on D_{al} must equal the first index of A_{am} . This involves reorienting the indices of D_{al} by using the transpose. Hence the product should be written as $(D_{la})^t A_{am}$, where the superscript t refers to the transpose.

$$\sum_{ijk} \Lambda_{imnij}^e \phi_{ijk}^e = \quad (6.6.28)$$

$$\sum_a (D_{1a})^t [(C_{11})_{amn}^e B_{amn}^{re} + (C_{12})_{amn}^e B_{amn}^{se} + (C_{13})_{amn}^e B_{amn}^{te}] +$$

$$\sum_b [(C_{12})_{bn}^e B_{bn}^{re} + (C_{22})_{bn}^e B_{bn}^{se} + (C_{23})_{bn}^e B_{bn}^{te}] D_{bn}^e +$$

$$\sum_c [(C_{13})_{mc}^e B_{mc}^{re} + (C_{23})_{mc}^e B_{mc}^{se} + (C_{33})_{mc}^e B_{mc}^{te}] D_{cn}^e.$$

This equation applies throughout a single element. Equation (6.6.7) summed over all elements gives

$$\sum_{e=1}^E \sum_{ijk} [\Lambda_{imnij}^e - \lambda^2 \Pi_{imnij}^e] \phi_{ijk}^e =$$

$$\sum_{e=1}^E \sum_{ijk} \Pi_{imnij}^e F_{ijk}^e. \quad (6.6.29)$$

This matrix expression for the unknown expansion coefficients ϕ_{imn}^e appears in the standard form, $Ax=B$. These coefficients represent the velocity at the nodes. We use this expression in a global node numbering system, where the global nodes lying on faces shared between adjacent elements receive a single label and contain a single value for each variable, though several elements may contribute. The assembly process, referred to as 'direct stiffness', properly accounts for the contributions from several elements.

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APPENDIX A

CO-ORDINATE TRANSFORMATION

A.1 Global and Local Co-ordinates

We decompose the given domain into arbitrarily shaped six-sided elements, we then transform these elements from the global co-ordinate system which applies to the entire domain to a local co-ordinate system within each element. The elements in physical space transform into cubes in local space, with local co-ordinates ranging between ± 1 . Since the physical equations apply in global space, we must develop a method for representing spatial derivatives and integrals in the local system. Specifically, we require a method to transfer from a co-ordinate system (x_1, x_2, x_3) to a system (ξ_1, ξ_2, ξ_3) .

Assuming an expression such as

$$x_i = x_i(\xi_1, \xi_2, \xi_3) \quad (\text{A.1.1})$$

exists between the two co-ordinate systems, the total derivative of x_i appears as

$$dx_i = \frac{\partial x_i}{\partial \xi_j} d\xi_j = \frac{\partial x_i}{\partial \xi_1} d\xi_1 + \frac{\partial x_i}{\partial \xi_2} d\xi_2 + \frac{\partial x_i}{\partial \xi_3} d\xi_3. \quad (\text{A.1.2})$$

Expressing this relation as a vector by letting $d\mathbf{x}^i$ equal the vector with components $(\partial x_i / \partial \xi_j) d\xi_j$, changes the total differentials into

$$d\mathbf{x}^1 = \frac{\partial x_1}{\partial \xi_1} d\xi_1 \mathbf{e}_1 + \frac{\partial x_1}{\partial \xi_2} d\xi_2 \mathbf{e}_2 + \frac{\partial x_1}{\partial \xi_3} d\xi_3 \mathbf{e}_3, \quad (\text{A.1.3})$$

$$d\mathbf{x}^2 = \frac{\partial x_2}{\partial \xi_1} d\xi_1 \mathbf{e}_1 + \frac{\partial x_2}{\partial \xi_2} d\xi_2 \mathbf{e}_2 + \frac{\partial x_2}{\partial \xi_3} d\xi_3 \mathbf{e}_3, \quad (\text{A.1.4})$$

and
$$d\mathbf{x}^3 = \frac{\partial x_3}{\partial \xi_1} d\xi_1 \mathbf{e}_1 + \frac{\partial x_3}{\partial \xi_2} d\xi_2 \mathbf{e}_2 + \frac{\partial x_3}{\partial \xi_3} d\xi_3 \mathbf{e}_3. \quad (\text{A.1.5})$$

We require differentials in vector form since the various surface integrals encountered in the analysis contain differential areas pointed in the surface normal direction.

A.2 Transform Between Global and Local Co-ordinates

Equation (A.1.2) represents a valid procedure for transforming from the

global co-ordinates (x,y,z) to the local co-ordinates (r,s,t) . In matrix form this transformation equals

$$\begin{bmatrix} dx \\ dy \\ dz \end{bmatrix} = \begin{bmatrix} x_r & x_s & x_t \\ y_r & y_s & y_t \\ z_r & z_s & z_t \end{bmatrix} \begin{bmatrix} dr \\ ds \\ dt \end{bmatrix} = [J] \begin{bmatrix} dr \\ ds \\ dt \end{bmatrix}, \quad (\text{A.2.1})$$

where the Jacobian, $[J]$, equals

$$[J] = \begin{bmatrix} x_r & x_s & x_t \\ y_r & y_s & y_t \\ z_r & z_s & z_t \end{bmatrix}. \quad (\text{A.2.2})$$

Subscripts refer to partial derivatives with respect to the local co-ordinates. The inverse transform, whereby the local co-ordinates appear in terms of global ones, equals

$$\begin{bmatrix} dr \\ ds \\ dt \end{bmatrix} = [J^{-1}] \begin{bmatrix} dx \\ dy \\ dz \end{bmatrix}. \quad (\text{A.2.3})$$

The inverse of the Jacobian equals

$$[J^{-1}] = \frac{1}{\det[J]} \begin{bmatrix} y_s z_t - y_t z_s & x_t z_s - x_s z_t & x_s y_t - x_t y_s \\ y_t z_r - y_r z_t & x_r z_t - x_t z_r & x_t y_r - x_r y_t \\ y_r z_s - y_s z_r & x_s z_r - x_r z_s & x_r y_s - x_s y_r \end{bmatrix}, \quad (\text{A.2.4})$$

which simplifies, upon introduction of

$$x_1 = y_s z_t - y_t z_s, \quad x_2 = y_t z_r - y_r z_t, \quad x_3 = y_r z_s - y_s z_r,$$

$$y_1 = x_t z_s - x_s z_t, \quad y_2 = x_r z_t - x_t z_r, \quad y_3 = x_s z_r - x_r z_s,$$

and

$$z_1 = x_s y_t - x_t y_s, \quad z_2 = x_t y_r - x_r y_t, \quad z_3 = x_r y_s - x_s y_r,$$

to

$$[J^{-1}] = \frac{1}{\det[J]} \begin{bmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \end{bmatrix}. \quad (\text{A.2.6})$$

Substituting into the inverse transform results in

$$\begin{bmatrix} dr \\ ds \\ dt \end{bmatrix} = \frac{1}{\det[J]} \begin{bmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \end{bmatrix} \begin{bmatrix} dx \\ dy \\ dz \end{bmatrix}, \quad (\text{A.2.7})$$

which represents a convenient method for computing total derivatives of local co-ordinates as functions of global differentials. Partial derivatives of the local co-ordinates occur when two of the global co-ordinates remain constant, or,

equivalently, by setting one or more of the differential quantities dx , dy , or dz equal to zero.

A.3 Volume Transformation

The variational form of the equations of motion contain volume integrals in physical space; however, the expansion functions only apply in transform space. Consequently, we require a transformation procedure for conversions between the two systems.

If the vector dx^i represents a differential length in the global system, a differential volume equals

$$dV = dx^1 \cdot (dx^2 \times dx^3). \quad (A.3.1)$$

Using the previously derived expressions for the vectors dx^i gives

$$dV = \epsilon_{ijk} \frac{\partial x_1}{\partial \xi_i} d\xi_i \frac{\partial x_2}{\partial \xi_j} d\xi_j \frac{\partial x_3}{\partial \xi_k} d\xi_k, \quad (A.3.2)$$

where ϵ_{ijk} equals the alternating unit tensor. Introducing the Jacobian gives

$$dV = \det[J] d\xi_1 d\xi_2 d\xi_3; \quad (A.3.3)$$

where the determinant of the Jacobian depends on

$$\begin{aligned} \det[J] d\xi_1 d\xi_2 d\xi_3 &= \epsilon_{ijk} \frac{\partial x_1}{\partial \xi_i} \frac{\partial x_2}{\partial \xi_j} \frac{\partial x_3}{\partial \xi_k} d\xi_i d\xi_j d\xi_k \\ &= \frac{\partial(x_1, x_2, x_3)}{\partial(\xi_1, \xi_2, \xi_3)} d\xi_1 d\xi_2 d\xi_3. \end{aligned} \quad (A.3.4)$$

We require

$$0 < |\det[J]| < \infty \quad (A.3.5)$$

for a proper transformation. With (A.3.3) we have a method for transforming volume integrals between the global and local co-ordinate systems. This transformation appears in the variational statement of the governing differential equations, or whenever a volume integral in the global system appears.

A.4 Partial Derivatives

The governing differential equations require partial derivatives of the

dependent variables in terms of the global co-ordinates. Since the global co-ordinates depend on the local co-ordinates, and vice versa, partial derivatives may appear as

$$\frac{\partial \varphi}{\partial x} = \frac{\partial \varphi}{\partial r} \frac{\partial r}{\partial x} + \frac{\partial \varphi}{\partial s} \frac{\partial s}{\partial x} + \frac{\partial \varphi}{\partial t} \frac{\partial t}{\partial x}, \quad (\text{A.4.1})$$

$$\frac{\partial \varphi}{\partial y} = \frac{\partial \varphi}{\partial r} \frac{\partial r}{\partial y} + \frac{\partial \varphi}{\partial s} \frac{\partial s}{\partial y} + \frac{\partial \varphi}{\partial t} \frac{\partial t}{\partial y}, \quad (\text{A.4.2})$$

and
$$\frac{\partial \varphi}{\partial z} = \frac{\partial \varphi}{\partial r} \frac{\partial r}{\partial z} + \frac{\partial \varphi}{\partial s} \frac{\partial s}{\partial z} + \frac{\partial \varphi}{\partial t} \frac{\partial t}{\partial z}. \quad (\text{A.4.3})$$

The partial derivatives of local co-ordinates depend on (A.2.7). For example, the partial derivative $\partial r / \partial x$ equals

$$\frac{\partial r}{\partial x} = \left. \frac{dr}{dx} \right|_{y,z} = \frac{1}{\det[J]} x_1. \quad (\text{A.4.4})$$

Using similar expressions for the other derivatives gives

$$\frac{\partial \varphi}{\partial x} = \frac{x_1}{\det[J]} \frac{\partial \varphi}{\partial r} + \frac{x_2}{\det[J]} \frac{\partial \varphi}{\partial s} + \frac{x_3}{\det[J]} \frac{\partial \varphi}{\partial t}, \quad (\text{A.4.5})$$

$$\frac{\partial \varphi}{\partial y} = \frac{y_1}{\det[J]} \frac{\partial \varphi}{\partial r} + \frac{y_2}{\det[J]} \frac{\partial \varphi}{\partial s} + \frac{y_3}{\det[J]} \frac{\partial \varphi}{\partial t}, \quad (\text{A.4.6})$$

and
$$\frac{\partial \varphi}{\partial z} = \frac{z_1}{\det[J]} \frac{\partial \varphi}{\partial r} + \frac{z_2}{\det[J]} \frac{\partial \varphi}{\partial s} + \frac{z_3}{\det[J]} \frac{\partial \varphi}{\partial t}. \quad (\text{A.4.7})$$

Expressions such as these appear whenever we represent partial derivatives of the dependent variables in transform space.

A.5 Partial Derivatives Using Spectral Expansions

The approximation procedure expresses the dependent variables as a truncated series of interpolating functions and coefficients. Therefore, expressions such as (A.4.5), containing the dependent variable φ , actually contain a series of coefficients and functions which depend on the local co-ordinates. Our method uses interpolating functions based on the Legendre polynomials. For example, the one-dimensional interpolation function of order n for the dependent variable φ equals

$$I_n \varphi = \sum_{k=0}^n \tilde{\varphi}_k \psi_k(r). \quad (\text{A.5.1})$$

which contains the interpolating functions, $\{\psi_k(r), k=0,1,\dots,n\}$, and coefficients,

$\tilde{\varphi}_k$. The derivative of φ with respect to the local variable r appears as

$$D_n \varphi(r) = \sum_{k=0}^n \tilde{\varphi}_k \frac{d}{dr} [\psi_k(r)]. \quad (\text{A.5.2})$$

In the current formulation, we compute the derivatives at the nodes and not between nodes. Evaluating the derivative at r_a gives

$$D_n \varphi(r_a) = \sum_{k=0}^n \tilde{\varphi}_k D_{ak}, \quad (\text{A.5.3})$$

where $\frac{d}{dr} [\psi_k(r)]_{r=a} \equiv D_{ak}$ represents the derivative of the expansion function ψ_k with respect to the local co-ordinate r at node r_a . Substituting similar expressions for the other partial derivatives in (A.4.5) gives

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial x}\right)_{abc}^e &= \left(\frac{x_1}{\det[\mathbf{J}]}\right)_{abc}^e \sum_{ijk} \tilde{\varphi}_{ijk}^e D_{ai} \psi_j(s_b) \psi_k(t_c) \\ &+ \left(\frac{x_2}{\det[\mathbf{J}]}\right)_{abc}^e \sum_{ijk} \tilde{\varphi}_{ijk}^e \psi_i(r_a) D_{bj} \psi_k(t_c) + \left(\frac{x_3}{\det[\mathbf{J}]}\right)_{abc}^e \sum_{ijk} \tilde{\varphi}_{ijk}^e \psi_i(r_a) \psi_j(s_b) D_{ck}. \end{aligned} \quad (\text{A.5.4})$$

The superscript e represents the element number, while the subscripts abc stand for the spatial node under consideration. Since the interpolating polynomials satisfy $\psi_i(r_a) = \delta_{ai}$, the partial derivative expressions reduce to

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial x}\right)_{abc}^e &= \left(\frac{x_1}{\det[\mathbf{J}]}\right)_{abc}^e \sum_i \tilde{\varphi}_{ibc}^e D_{ai} + \left(\frac{x_2}{\det[\mathbf{J}]}\right)_{abc}^e \sum_j \tilde{\varphi}_{ajc}^e D_{bj} + \left(\frac{x_3}{\det[\mathbf{J}]}\right)_{abc}^e \sum_k \tilde{\varphi}_{abk}^e D_{ck}, \\ \left(\frac{\partial \varphi}{\partial y}\right)_{abc}^e &= \left(\frac{y_1}{\det[\mathbf{J}]}\right)_{abc}^e \sum_i \tilde{\varphi}_{ibc}^e D_{ai} + \left(\frac{y_2}{\det[\mathbf{J}]}\right)_{abc}^e \sum_j \tilde{\varphi}_{ajc}^e D_{bj} + \left(\frac{y_3}{\det[\mathbf{J}]}\right)_{abc}^e \sum_k \tilde{\varphi}_{abk}^e D_{ck}, \\ \left(\frac{\partial \varphi}{\partial z}\right)_{abc}^e &= \left(\frac{z_1}{\det[\mathbf{J}]}\right)_{abc}^e \sum_i \tilde{\varphi}_{ibc}^e D_{ai} + \left(\frac{z_2}{\det[\mathbf{J}]}\right)_{abc}^e \sum_j \tilde{\varphi}_{ajc}^e D_{bj} + \left(\frac{z_3}{\det[\mathbf{J}]}\right)_{abc}^e \sum_k \tilde{\varphi}_{abk}^e D_{ck}. \end{aligned} \quad (\text{G.5.5})$$

These equations represent the partial derivatives of the dependent variable, φ , at the nodal points. At this point we impose no restriction on the location of a node within an element, i.e., the node may lie in the interior or on the surface of an element. The next section computes derivatives along element faces by applying (A.5.5) to nodes lying along the surface.

A.6 Derivatives Along Element Faces

The calculation of surface stresses requires derivatives along element faces. The equations for derivatives at any node (a,b,c) simplify along the element

surface since one of the indices remains fixed while the other two vary. This results in a set of expressions for each of the six element faces:

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial x}\right)_{ab1}^e &= \left(\frac{x_1}{\det[J]}\right)_{ab1}^e \sum_i \tilde{\varphi}_{ib1}^e D_{ai} + \left(\frac{x_2}{\det[J]}\right)_{ab1}^e \sum_j \tilde{\varphi}_{aj1}^e D_{bj} \\ &\quad + \left(\frac{x_3}{\det[J]}\right)_{ab1}^e \sum_k \tilde{\varphi}_{abk}^e D_{ik}, \end{aligned} \quad (A.6.1)$$

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial y}\right)_{ab1}^e &= \left(\frac{y_1}{\det[J]}\right)_{ab1}^e \sum_i \tilde{\varphi}_{ib1}^e D_{ai} + \left(\frac{y_2}{\det[J]}\right)_{ab1}^e \sum_j \tilde{\varphi}_{aj1}^e D_{bj} \\ &\quad + \left(\frac{y_3}{\det[J]}\right)_{ab1}^e \sum_k \tilde{\varphi}_{abk}^e D_{ik} \end{aligned}$$

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial z}\right)_{ab1}^e &= \left(\frac{z_1}{\det[J]}\right)_{ab1}^e \sum_i \tilde{\varphi}_{ib1}^e D_{ai} + \left(\frac{z_2}{\det[J]}\right)_{ab1}^e \sum_j \tilde{\varphi}_{aj1}^e D_{bj} \\ &\quad + \left(\frac{z_3}{\det[J]}\right)_{ab1}^e \sum_k \tilde{\varphi}_{abk}^e D_{ik}, \text{ along the side at } t = -1; \end{aligned}$$

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial x}\right)_{ajtc}^e &= \left(\frac{x_1}{\det[J]}\right)_{ajtc}^e \sum_i \tilde{\varphi}_{ijtc}^e D_{ai} + \left(\frac{x_2}{\det[J]}\right)_{ajtc}^e \sum_j \tilde{\varphi}_{ajc}^e D_{jtj} \\ &\quad + \left(\frac{x_3}{\det[J]}\right)_{ajtc}^e \sum_k \tilde{\varphi}_{ajtk}^e D_{ck} \end{aligned} \quad (A.6.2)$$

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial y}\right)_{ajtc}^e &= \left(\frac{y_1}{\det[J]}\right)_{ajtc}^e \sum_i \tilde{\varphi}_{ijtc}^e D_{ai} + \left(\frac{y_2}{\det[J]}\right)_{ajtc}^e \sum_j \tilde{\varphi}_{ajc}^e D_{jtj} \\ &\quad + \left(\frac{y_3}{\det[J]}\right)_{ajtc}^e \sum_k \tilde{\varphi}_{ajtk}^e D_{ck} \end{aligned}$$

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial z}\right)_{ajtc}^e &= \left(\frac{z_1}{\det[J]}\right)_{ajtc}^e \sum_i \tilde{\varphi}_{ijtc}^e D_{ai} + \left(\frac{z_2}{\det[J]}\right)_{ajtc}^e \sum_j \tilde{\varphi}_{ajc}^e D_{jtj} \\ &\quad + \left(\frac{z_3}{\det[J]}\right)_{ajtc}^e \sum_k \tilde{\varphi}_{ajtk}^e D_{ck}, \text{ along the side at } s=1; \end{aligned}$$

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial x}\right)_{abkt}^e &= \left(\frac{x_1}{\det[J]}\right)_{abkt}^e \sum_i \tilde{\varphi}_{ibkt}^e D_{ai} + \left(\frac{x_2}{\det[J]}\right)_{abkt}^e \sum_j \tilde{\varphi}_{ajkt}^e D_{bj} \\ &\quad + \left(\frac{x_3}{\det[J]}\right)_{abkt}^e \sum_k \tilde{\varphi}_{abk}^e D_{ktk} \end{aligned} \quad (A.6.3)$$

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial y}\right)_{abkt}^e &= \left(\frac{y_1}{\det[J]}\right)_{abkt}^e \sum_i \tilde{\varphi}_{ibkt}^e D_{ai} + \left(\frac{y_2}{\det[J]}\right)_{abkt}^e \sum_j \tilde{\varphi}_{ajkt}^e D_{bj} \\ &\quad + \left(\frac{y_3}{\det[J]}\right)_{abkt}^e \sum_k \tilde{\varphi}_{abk}^e D_{ktk} \end{aligned}$$

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial z}\right)_{abkt}^e &= \left(\frac{z_1}{\det[J]}\right)_{abkt}^e \sum_i \tilde{\varphi}_{ibkt}^e D_{ai} + \left(\frac{z_2}{\det[J]}\right)_{abkt}^e \sum_j \tilde{\varphi}_{ajkt}^e D_{bj} \\ &\quad + \left(\frac{z_3}{\det[J]}\right)_{abkt}^e \sum_k \tilde{\varphi}_{abk}^e D_{ktk}, \text{ along the side } t=1; \end{aligned}$$

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial x}\right)_{a1c}^e &= \left(\frac{x_1}{\det[J]}\right)_{a1c}^e \sum_i \tilde{\varphi}_{i1c}^e D_{ai} + \left(\frac{x_2}{\det[J]}\right)_{a1c}^e \sum_j \tilde{\varphi}_{ajc}^e D_{1j} \\ &\quad + \left(\frac{x_3}{\det[J]}\right)_{a1c}^e \sum_k \tilde{\varphi}_{a1k}^e D_{ck} \end{aligned} \quad (A.6.4)$$

$$\begin{aligned} \left(\frac{\partial \varphi}{\partial y}\right)_{a1c}^e &= \left(\frac{y_1}{\det[J]}\right)_{a1c}^e \sum_i \tilde{\varphi}_{i1c}^e D_{ai} + \left(\frac{y_2}{\det[J]}\right)_{a1c}^e \sum_j \tilde{\varphi}_{ajc}^e D_{1j} \\ &\quad + \left(\frac{y_3}{\det[J]}\right)_{a1c}^e \sum_k \tilde{\varphi}_{a1k}^e D_{ck} \end{aligned}$$

$$\left(\frac{\partial \varphi}{\partial z}\right)_{a1c}^e = \left(\frac{z_1}{\det[J]}\right)_{a1c}^e \sum_i \tilde{\varphi}_{i1c}^e D_{ai} + \left(\frac{z_2}{\det[J]}\right)_{a1c}^e \sum_j \tilde{\varphi}_{ajc}^e D_{1j}$$

$$\begin{aligned}
& + \frac{z_3}{\det[\mathbf{J}]} \bar{\varphi}_{a1c}^e \sum_k \bar{\varphi}_{a1k}^e D_{ck}, \text{ along the side } s = -1; \\
\left(\frac{\partial \varphi}{\partial x}\right)_{i bc}^e &= \left(\frac{x_1}{\det[\mathbf{J}]} \right)_{i bc}^e \sum_i \bar{\varphi}_{i bc}^e D_{1i} + \left(\frac{x_2}{\det[\mathbf{J}]} \right)_{i bc}^e \sum_j \bar{\varphi}_{i jc}^e D_{bj} \\
& + \left(\frac{x_3}{\det[\mathbf{J}]} \right)_{i bc}^e \sum_k \bar{\varphi}_{i bk}^e D_{ck} \\
\left(\frac{\partial \varphi}{\partial y}\right)_{i bc}^e &= \left(\frac{y_1}{\det[\mathbf{J}]} \right)_{i bc}^e \sum_i \bar{\varphi}_{i bc}^e D_{1i} + \left(\frac{y_2}{\det[\mathbf{J}]} \right)_{i bc}^e \sum_j \bar{\varphi}_{i jc}^e D_{bj} \\
& + \left(\frac{y_3}{\det[\mathbf{J}]} \right)_{i bc}^e \sum_k \bar{\varphi}_{i bk}^e D_{ck}
\end{aligned} \tag{A.6.5}$$

$$\begin{aligned}
\left(\frac{\partial \varphi}{\partial z}\right)_{i bc}^e &= \left(\frac{z_1}{\det[\mathbf{J}]} \right)_{i bc}^e \sum_i \bar{\varphi}_{i bc}^e D_{1i} + \left(\frac{z_2}{\det[\mathbf{J}]} \right)_{i bc}^e \sum_j \bar{\varphi}_{i jc}^e D_{bj} \\
& + \left(\frac{z_3}{\det[\mathbf{J}]} \right)_{i bc}^e \sum_k \bar{\varphi}_{i bk}^e D_{ck}, \text{ along the side } r = -1; \text{ and} \\
\left(\frac{\partial \varphi}{\partial x}\right)_{i t bc}^e &= \left(\frac{x_1}{\det[\mathbf{J}]} \right)_{i t bc}^e \sum_i \bar{\varphi}_{i bc}^e D_{1i} + \left(\frac{x_2}{\det[\mathbf{J}]} \right)_{i t bc}^e \sum_j \bar{\varphi}_{i t jc}^e D_{bj} \\
& + \left(\frac{x_3}{\det[\mathbf{J}]} \right)_{i t bc}^e \sum_k \bar{\varphi}_{i t bk}^e D_{ck} \\
\left(\frac{\partial \varphi}{\partial y}\right)_{i t bc}^e &= \left(\frac{y_1}{\det[\mathbf{J}]} \right)_{i t bc}^e \sum_i \bar{\varphi}_{i bc}^e D_{1i} + \left(\frac{y_2}{\det[\mathbf{J}]} \right)_{i t bc}^e \sum_j \bar{\varphi}_{i t jc}^e D_{bj} \\
& + \left(\frac{y_3}{\det[\mathbf{J}]} \right)_{i t bc}^e \sum_k \bar{\varphi}_{i t bk}^e D_{ck} \\
\left(\frac{\partial \varphi}{\partial z}\right)_{i t bc}^e &= \left(\frac{z_1}{\det[\mathbf{J}]} \right)_{i t bc}^e \sum_i \bar{\varphi}_{i bc}^e D_{1i} + \left(\frac{z_2}{\det[\mathbf{J}]} \right)_{i t bc}^e \sum_j \bar{\varphi}_{i t jc}^e D_{bj} \\
& + \left(\frac{z_3}{\det[\mathbf{J}]} \right)_{i t bc}^e \sum_k \bar{\varphi}_{i t bk}^e D_{ck}, \text{ along the side } r = 1.
\end{aligned} \tag{A.6.6}$$

A.7 Surface Integrals

Often surface integrals involving the differential area vector appear in boundary conditions and computations of surface stresses inter alia. According to (A.1.3) through (A.1.5), the transformation between global co-ordinates (x, y, z) and local co-ordinates (r, s, t) equals

$$dx = \frac{\partial x}{\partial r} dr + \frac{\partial x}{\partial s} ds + \frac{\partial x}{\partial t} dt, \tag{A.7.1}$$

$$dy = \frac{\partial y}{\partial r} dr + \frac{\partial y}{\partial s} ds + \frac{\partial y}{\partial t} dt, \tag{A.7.2}$$

and

$$dz = \frac{\partial z}{\partial r} dr + \frac{\partial z}{\partial s} ds + \frac{\partial z}{\partial t} dt. \tag{A.7.3}$$

In the local co-ordinate system, the element surface depends on two of the three local variables while the third remains fixed. For example, along side one co-ordinates r and s vary, while co-ordinate t equals -1 . Hence, the transformation along side one appears as

$$dx^1 = \frac{\partial x}{\partial r} dr e_r + \frac{\partial x}{\partial s} ds e_s, \quad (A.7.4)$$

$$dy^1 = \frac{\partial y}{\partial r} dr e_r + \frac{\partial y}{\partial s} ds e_s, \quad (A.7.5)$$

and
$$dz^1 = \frac{\partial z}{\partial r} dr e_r + \frac{\partial z}{\partial s} ds e_s, \quad (A.7.6)$$

where here the superscript refers to side one and not direction one as in (A.1.3).

After integrating these relations, expressions for the physical co-ordinates in terms of the local co-ordinates along the surface appear:

$$x^1 = x(r,s), \quad (A.7.7)$$

$$y^1 = y(r,s), \quad (A.7.8)$$

and
$$z^1 = z(r,s). \quad (A.7.9)$$

Let $R^1 = x^1 e_x + y^1 e_y + z^1 e_z$ represent a position vector describing the location of any point along surface one. Substituting the previous expressions for the physical co-ordinates into this position vector gives

$$R^1 = x(r,s) e_x + y(r,s) e_y + z(r,s) e_z. \quad (A.7.10)$$

A differential area vector in the normal direction to the surface corresponding to a differential change in the local co-ordinates r and s equals

$$dA^1 = - \left(\frac{\partial R}{\partial r} \times \frac{\partial R}{\partial s} \right) dr ds. \quad (A.7.11)$$

The minus sign indicates that the area vector points in the local co-ordinate direction $-e_t$. We can write the two partial derivatives as

$$\frac{\partial R}{\partial r} = \frac{\partial R}{\partial x} \frac{\partial x}{\partial r} e_x + \frac{\partial R}{\partial y} \frac{\partial y}{\partial r} e_y + \frac{\partial R}{\partial z} \frac{\partial z}{\partial r} e_z, \quad (A.7.12)$$

and
$$\frac{\partial R}{\partial s} = \frac{\partial R}{\partial x} \frac{\partial x}{\partial s} e_x + \frac{\partial R}{\partial y} \frac{\partial y}{\partial s} e_y + \frac{\partial R}{\partial z} \frac{\partial z}{\partial s} e_z. \quad (A.7.13)$$

Using (A.7.10) reduces these expressions to

$$\frac{\partial R}{\partial r} = x_r e_x + y_r e_y + z_r e_z, \quad (A.7.14)$$

and
$$\frac{\partial R}{\partial s} = x_s e_x + y_s e_y + z_s e_z. \quad (A.7.15)$$

Substituting these expressions into dA^1 and taking the cross-product gives

$$dA^1 = - [(y_r z_s - z_r y_s) e_x + (z_r x_s - x_r z_s) e_y +$$

$$(x_r y_s - y_r x_s) e_z] dr ds, \quad (\text{A.7.16})$$

or, using the simplified notation of (A.2.5)

$$dA^1 = -(x_3 e_x + y_3 e_y + z_3 e_z) dr ds. \quad (\text{A.7.17})$$

Similar expressions for sides two through six equal

$$dA^2 = (x_2 e_x + y_2 e_y + z_2 e_z) dr dt, \quad (\text{A.7.18})$$

$$dA^3 = (x_3 e_x + y_3 e_y + z_3 e_z) dr ds, \quad (\text{A.7.19})$$

$$dA^4 = -(x_2 e_x + y_2 e_y + z_2 e_z) dr dt, \quad (\text{A.7.20})$$

$$dA^5 = -(x_1 e_x + y_1 e_y + z_1 e_z) ds dt, \quad (\text{A.7.21})$$

and $dA^6 = (x_1 e_x + y_1 e_y + z_1 e_z) ds dt. \quad (\text{A.7.22})$

Expressions such as these will appear whenever we compute surface integrals.

APPENDIX B

SURFACE FORCE AND MOMENT CALCULATION

B.1 Background

Fluid flowing past solid boundaries develops surface stresses which lead to surface forces and moments after integration over the surface area. The elements located adjacent to these surfaces contain flow-field information necessary for surface stress calculations. Let dA equal a differential area on the element surface with unit normal vector \mathbf{n} . Let the force per unit area due to the fluid stresses on this surface equal $\mathbf{t}(\mathbf{n})$. Then, the total force on a finite surface, $\partial\Omega$, results from integrating the contributions from all the differential elements:

$$\mathbf{F} = \iint_{\partial\Omega} \mathbf{t}(\mathbf{n}) dA. \quad (\text{B.1.1})$$

Similarly, the total moment about a given point due to the surface forces equals

$$\mathbf{M} = \iint_{\partial\Omega} \boldsymbol{\chi} \times \mathbf{t}(\mathbf{n}) dA, \quad (\text{B.1.2})$$

where $\boldsymbol{\chi}$ represents the distance between the surface element and the point about which the moment is taken. Let σ_{ji} denote the i^{th} component of $\mathbf{t}(\mathbf{j})$, and let $\mathbf{t}(\mathbf{n})_i$ denote the i^{th} component of $\mathbf{t}(\mathbf{n})$. Whence

$$\mathbf{t}(\mathbf{n})_i = \sigma_{ji} n_j, \quad (\text{B.1.3})$$

where the stress tensor equals

$$\underline{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}. \quad (\text{B.1.4})$$

Since $\mathbf{t}(\mathbf{n})$ represents a vector and \mathbf{n} represents a unit vector independent of the σ_{ji} , we require

$$\mathbf{t}(\mathbf{n}) = \mathbf{n} \cdot \underline{\sigma}. \quad (\text{B.1.5})$$

This equation represents the force per unit area due to fluid stresses on a surface with unit normal vector \mathbf{n} . When this expression replaces $\mathbf{t}(\mathbf{n})$ in the force and

moment integrals, terms such as $\mathbf{n} \cdot \underline{\sigma} dA$ and $\chi^*(\mathbf{n} \cdot \underline{\sigma}) dA$ arise. Since dA represents a scalar, we may write these expressions as $\mathbf{n} dA \cdot \underline{\sigma}$ and $\chi^*(\mathbf{n} dA \cdot \underline{\sigma})$. We developed expressions for $\mathbf{n} dA$ along each of the six element faces in appendix A. We still need, however, an expression for the stress tensor.

B.2 Incompressible Stress Tensor

In Cartesian co-ordinates the diagonal components of the incompressible flow stress tensor equal

$$\sigma_{xx} = -p + 2\mu \frac{\partial u}{\partial x}, \quad \sigma_{yy} = -p + 2\mu \frac{\partial v}{\partial y},$$

and

$$\sigma_{zz} = -p + 2\mu \frac{\partial w}{\partial z}, \quad (\text{B.2.1})$$

while the off diagonal terms equal

$$\sigma_{xy} = \sigma_{yx} = \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right), \quad (\text{B.2.2})$$

$$\sigma_{xz} = \sigma_{zx} = \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right), \quad (\text{B.2.3})$$

and

$$\sigma_{yz} = \sigma_{zy} = \mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right). \quad (\text{B.2.4})$$

B.3 Surface Force

As indicated in §B.1, the force over a surface $\partial\Omega$ due to the fluid stresses equals

$$\mathbf{F} = \iint_{\partial\Omega} \mathbf{t}(\mathbf{n}) dA = \iint_{\partial\Omega} \mathbf{n} \cdot \underline{\sigma} dA. \quad (\text{B.3.1})$$

The components of the force in the global (x, y, z) system equal

$$F_x = \iint_{\partial\Omega} (\sigma_{xx} n_x + \sigma_{yx} n_y + \sigma_{zx} n_z) dA, \quad (\text{B.3.2})$$

$$F_y = \iint_{\partial\Omega} (\sigma_{xy} n_x + \sigma_{yy} n_y + \sigma_{zy} n_z) dA, \quad (\text{B.3.3})$$

and

$$F_z = \iint_{\partial\Omega} (\sigma_{xz} n_x + \sigma_{yz} n_y + \sigma_{zz} n_z) dA. \quad (\text{B.3.4})$$

Since $n_x dA$, $n_y dA$, and $n_z dA$ represent the projection of dA onto the planes perpendicular to the global co-ordinate axes, we may write $n_x dA = \mathbf{e}_x \cdot d\mathbf{A}$, $n_y dA = \mathbf{e}_y \cdot d\mathbf{A}$ and $n_z dA = \mathbf{e}_z \cdot d\mathbf{A}$. Substituting these expressions into the force

components gives

$$F_x = \iint_{\partial\Omega} (\sigma_{xx}e_x + \sigma_{yx}e_y + \sigma_{zx}e_z) \cdot dA, \quad (B.3.5)$$

$$F_y = \iint_{\partial\Omega} (\sigma_{xy}e_x + \sigma_{yy}e_y + \sigma_{zy}e_z) \cdot dA, \quad (B.3.6)$$

and
$$F_z = \iint_{\partial\Omega} (\sigma_{xz}e_x + \sigma_{yz}e_y + \sigma_{zz}e_z) \cdot dA. \quad (B.3.7)$$

The forces along side one, where $dA^1 = -(x_3e_x + y_3e_y + z_3e_z)drds$, equal

$$F_x^1 = - \iint_{\partial\Omega^1} (\sigma_{xx}x_3 + \sigma_{yx}y_3 + \sigma_{zx}z_3)drds. \quad (B.3.8)$$

$$F_y^1 = - \iint_{\partial\Omega^1} (\sigma_{xy}x_3 + \sigma_{yy}y_3 + \sigma_{zy}z_3)drds, \quad (B.3.9)$$

and
$$F_z^1 = - \iint_{\partial\Omega^1} (\sigma_{xz}x_3 + \sigma_{yz}y_3 + \sigma_{zz}z_3)drds. \quad (B.3.10)$$

On the local level, the surface of integration reduces to a square with sides ranging between ± 1 . Using the spectral collocation approximation allows an expression for the force F_x^1 as

$$F_x^{1e} = - \sum_{ij} \int_{-1}^1 \int_{-1}^1 (\sigma_{xx}x_3 + \sigma_{yx}y_3 + \sigma_{zx}z_3)_{ij1}^e \psi_i(r) \psi_j(s) drds, \quad (B.3.11)$$

where the expression $(...)_{ij1}^e$ indicates that the terms within the parentheses depend on the local node ij_1 of element e . Integrating over the element surface gives

$$F_x^{1e} = - \sum_{ij} (\sigma_{xx}x_3 + \sigma_{yx}y_3 + \sigma_{zx}z_3)_{ij1}^e w_i w_j. \quad (B.3.12)$$

In a similar manner, the y and z components appear as

$$F_y^{1e} = - \sum_{ij} (\sigma_{xy}x_3 + \sigma_{yy}y_3 + \sigma_{zy}z_3)_{ij1}^e w_i w_j \quad (B.3.13)$$

and
$$F_z^{1e} = - \sum_{ij} (\sigma_{xz}x_3 + \sigma_{yz}y_3 + \sigma_{zz}z_3)_{ij1}^e w_i w_j. \quad (B.3.14)$$

The forces on faces two through six equal

$$\begin{aligned} F_x^{2e} &= \sum_{ik} (\sigma_{xx}x_2 + \sigma_{yx}y_2 + \sigma_{zx}z_2)_{ikt}^e w_i w_k, \\ F_y^{2e} &= \sum_{ik} (\sigma_{xy}x_2 + \sigma_{yy}y_2 + \sigma_{zy}z_2)_{ikt}^e w_i w_k, \\ \text{and} \quad F_z^{2e} &= \sum_{ik} (\sigma_{xz}x_2 + \sigma_{yz}y_2 + \sigma_{zz}z_2)_{ikt}^e w_i w_k, \end{aligned} \quad (B.3.15)$$

on face two, where $dA=(x_2e_x+y_2e_y+z_2e_z)drdt$;

$$\begin{aligned} F_x^{3e} &= \sum_{ij} (\sigma_{xx}x_3 + \sigma_{yx}y_3 + \sigma_{zx}z_3) e_{ijk} w_i w_j, \\ F_y^{3e} &= \sum_{ij} (\sigma_{xy}x_3 + \sigma_{yy}y_3 + \sigma_{zy}z_3) e_{ijk} w_i w_j, \\ \text{and} \quad F_z^{3e} &= \sum_{ij} (\sigma_{xz}x_3 + \sigma_{yz}y_3 + \sigma_{zz}z_3) e_{ijk} w_i w_j, \end{aligned} \quad (B.3.16)$$

on face three, where $dA=(x_3e_x+y_3e_y+z_3e_z)drds$;

$$\begin{aligned} F_x^{4e} &= \sum_{ik} (\sigma_{xx}x_2 + \sigma_{yx}y_2 + \sigma_{zx}z_2) e_{ikj} w_i w_k, \\ F_y^{4e} &= \sum_{ik} (\sigma_{xy}x_2 + \sigma_{yy}y_2 + \sigma_{zy}z_2) e_{ikj} w_i w_k, \\ \text{and} \quad F_z^{4e} &= \sum_{ik} (\sigma_{xz}x_2 + \sigma_{yz}y_2 + \sigma_{zz}z_2) e_{ikj} w_i w_k, \end{aligned} \quad (B.3.17)$$

on face four, where $dA=-(x_2e_x+y_2e_y+z_2e_z)drdt$;

$$\begin{aligned} F_x^{5e} &= \sum_{jk} (\sigma_{xx}x_1 + \sigma_{yx}y_1 + \sigma_{zx}z_1) e_{jki} w_j w_k, \\ F_y^{5e} &= \sum_{jk} (\sigma_{xy}x_1 + \sigma_{yy}y_1 + \sigma_{zy}z_1) e_{jki} w_j w_k, \\ \text{and} \quad F_z^{5e} &= \sum_{jk} (\sigma_{xz}x_1 + \sigma_{yz}y_1 + \sigma_{zz}z_1) e_{jki} w_j w_k, \end{aligned} \quad (B.3.18)$$

on face five, where $dA=-(x_1e_x+y_1e_y+z_1e_z)dsdt$; and

$$\begin{aligned} F_x^{6e} &= \sum_{jk} (\sigma_{xx}x_1 + \sigma_{yx}y_1 + \sigma_{zx}z_1) e_{itjk} w_j w_k, \\ F_y^{6e} &= \sum_{jk} (\sigma_{xy}x_1 + \sigma_{yy}y_1 + \sigma_{zy}z_1) e_{itjk} w_j w_k, \\ \text{and} \quad F_z^{6e} &= \sum_{jk} (\sigma_{xz}x_1 + \sigma_{yz}y_1 + \sigma_{zz}z_1) e_{itjk} w_j w_k, \end{aligned} \quad (B.3.19)$$

on face six, where $dA=(x_1e_x+y_1e_y+z_1e_z)dsdt$. Note that when any of the subscripts ijk equals 1, we refer to the node at the face corresponding to rst equal to -1 , and when any of the ijk equals it , jt , or kt , we refer to the node at the face corresponding to rst equal to 1. Also, the basis functions integrated over the local co-ordinate domain, $w_i \equiv \int_{-1}^1 \psi_i(r) dr$, $w_j \equiv \int_{-1}^1 \psi_j(s) ds$, and $w_k \equiv \int_{-1}^1 \psi_k(t) dt$, differ when the number of nodes in the r , s , or t directions differ; consequently, we must remember that w_i refers to the r -direction, w_j refers to the s -direction, and w_k refers to the t -direction.

B.4 Surface Moment

The moment along a surface due to the fluid stresses appears as

$$\mathbf{M} = \iint_{\partial\Omega} \boldsymbol{\chi} \times \mathbf{n} \cdot \underline{\sigma} \, dA, \quad (\text{B.4.1})$$

where the moment "arm" equals $\boldsymbol{\chi} = \chi_x \mathbf{e}_x + \chi_y \mathbf{e}_y + \chi_z \mathbf{e}_z$. Substituting into (B.4.1) and performing the cross product yields the moment components in the global coordinates as

$$M_x = \iint_{\partial\Omega} [\chi_y(\sigma_{xz}n_x + \sigma_{yz}n_y + \sigma_{zz}n_z) - \chi_z(\sigma_{xy}n_x + \sigma_{yy}n_y + \sigma_{zy}n_z)] dA,$$

$$M_y = \iint_{\partial\Omega} [\chi_z(\sigma_{xx}n_x + \sigma_{yx}n_y + \sigma_{zx}n_z) - \chi_x(\sigma_{xz}n_x + \sigma_{yz}n_y + \sigma_{zz}n_z)] dA,$$

$$M_z = \iint_{\partial\Omega} [\chi_x(\sigma_{xy}n_x + \sigma_{yy}n_y + \sigma_{zy}n_z) - \chi_y(\sigma_{xx}n_x + \sigma_{yx}n_y + \sigma_{zx}n_z)] dA.$$

Using the same notation as in the surface force calculation gives

$$M_x = \iint_{\partial\Omega} [\chi_y(\sigma_{xz}\mathbf{e}_x + \sigma_{yz}\mathbf{e}_y + \sigma_{zz}\mathbf{e}_z) - \chi_z(\sigma_{xy}\mathbf{e}_x + \sigma_{yy}\mathbf{e}_y + \sigma_{zy}\mathbf{e}_z)] \cdot d\mathbf{A},$$

$$M_y = \iint_{\partial\Omega} [\chi_z(\sigma_{xx}\mathbf{e}_x + \sigma_{yx}\mathbf{e}_y + \sigma_{zx}\mathbf{e}_z) - \chi_x(\sigma_{xz}\mathbf{e}_x + \sigma_{yz}\mathbf{e}_y + \sigma_{zz}\mathbf{e}_z)] \cdot d\mathbf{A},$$

$$M_z = \iint_{\partial\Omega} [\chi_x(\sigma_{xy}\mathbf{e}_x + \sigma_{yy}\mathbf{e}_y + \sigma_{zy}\mathbf{e}_z) - \chi_y(\sigma_{xx}\mathbf{e}_x + \sigma_{yx}\mathbf{e}_y + \sigma_{zx}\mathbf{e}_z)] \cdot d\mathbf{A}.$$

(B.4.3)

For example, the x-component evaluated along side one, where

$d\mathbf{A} = -[x_3\mathbf{e}_x + y_3\mathbf{e}_y + z_3\mathbf{e}_z]drds$, equals

$$M_x^{1e} = -\int_{-1}^1 \int_{-1}^1 [\chi_y(\sigma_{xz}x_3 + \sigma_{yz}y_3 + \sigma_{zz}z_3) - \chi_z(\sigma_{xy}x_3 + \sigma_{yy}y_3 + \sigma_{zy}z_3)]^e drds.$$

Introducing the spectral expansion functions gives

$$M_x^{1e} = -\sum_{ij} \int_{-1}^1 \int_{-1}^1 [\chi_y(\sigma_{xz}x_3 + \sigma_{yz}y_3 + \sigma_{zz}z_3) - \chi_z(\sigma_{xy}x_3 + \sigma_{yy}y_3 + \sigma_{zy}z_3)]_{ij}^e \psi_i(\mathbf{r}) \psi_j(\mathbf{s}) drds. \quad (\text{B.4.4})$$

After integration we obtain

$$M_x^{1e} = -\sum_{ij} [\chi_y(\sigma_{xz}x_3 + \sigma_{yz}y_3 + \sigma_{zz}z_3) - \chi_z(\sigma_{xy}x_3 + \sigma_{yy}y_3 + \sigma_{zy}z_3)]_{ij}^e w_i w_j. \quad (\text{B.4.5})$$

In a similar manner, the y and z components appear as

$$M_y^{1e} = -\sum_{ij} [\chi_z(\sigma_{xx}x_3 + \sigma_{yx}y_3 + \sigma_{zx}z_3) - \chi_x(\sigma_{xz}x_3 + \sigma_{yz}y_3 + \sigma_{zz}z_3)] e_{ij1} w_i w_j,$$

$$M_z^{1e} = -\sum_{ij} [\chi_x(\sigma_{xy}x_3 + \sigma_{yy}y_3 + \sigma_{zy}z_3) - \chi_y(\sigma_{xx}x_3 + \sigma_{yx}y_3 + \sigma_{zx}z_3)] e_{ij1} w_i w_j.$$

The moments along faces two through six equal

$$M_x^{2e} = \sum_{ik} [\chi_y(\sigma_{xz}x_2 + \sigma_{yz}y_2 + \sigma_{zz}z_2) - \chi_z(\sigma_{xy}x_2 + \sigma_{yy}y_2 + \sigma_{zy}z_2)] e_{ikt} w_i w_k,$$

$$M_y^{2e} = \sum_{ik} [\chi_z(\sigma_{xx}x_2 + \sigma_{yx}y_2 + \sigma_{zx}z_2) - \chi_x(\sigma_{xz}x_2 + \sigma_{yz}y_2 + \sigma_{zz}z_2)] e_{ikt} w_i w_k,$$

$$M_z^{2e} = \sum_{ik} [\chi_x(\sigma_{xy}x_2 + \sigma_{yy}y_2 + \sigma_{zy}z_2) - \chi_y(\sigma_{xx}x_2 + \sigma_{yx}y_2 + \sigma_{zx}z_2)] e_{ikt} w_i w_k,$$

along face two, where $dA = (x_2 e_x + y_2 e_y + z_2 e_z) drdt$; (B.4.6)

$$M_x^{3e} = \sum_{ij} [\chi_y(\sigma_{xz}x_3 + \sigma_{yz}y_3 + \sigma_{zz}z_3) - \chi_z(\sigma_{xy}x_3 + \sigma_{yy}y_3 + \sigma_{zy}z_3)] e_{ijkt} w_i w_j,$$

$$M_y^{3e} = \sum_{ij} [\chi_z(\sigma_{xx}x_3 + \sigma_{yx}y_3 + \sigma_{zx}z_3) - \chi_x(\sigma_{xz}x_3 + \sigma_{yz}y_3 + \sigma_{zz}z_3)] e_{ijkt} w_i w_j,$$

$$M_z^{3e} = \sum_{ij} [\chi_x(\sigma_{xy}x_3 + \sigma_{yy}y_3 + \sigma_{zy}z_3) - \chi_y(\sigma_{xx}x_3 + \sigma_{yx}y_3 + \sigma_{zx}z_3)] e_{ijkt} w_i w_j,$$

along face three, where $dA = (x_3 e_x + y_3 e_y + z_3 e_z) drds$; (B.4.7)

$$M_x^{4e} = -\sum_{ik} [\chi_y(\sigma_{xz}x_2 + \sigma_{yz}y_2 + \sigma_{zz}z_2) - \chi_z(\sigma_{xy}x_2 + \sigma_{yy}y_2 + \sigma_{zy}z_2)] e_{ikl} w_i w_k,$$

$$M_y^{4e} = -\sum_{ik} [\chi_z(\sigma_{xx}x_2 + \sigma_{yx}y_2 + \sigma_{zx}z_2) - \chi_x(\sigma_{xz}x_2 + \sigma_{yz}y_2 + \sigma_{zz}z_2)] e_{ikl} w_i w_k,$$

$$M_z^{4e} = -\sum_{ik} [\chi_x(\sigma_{xy}x_2 + \sigma_{yy}y_2 + \sigma_{zy}z_2) - \chi_y(\sigma_{xx}x_2 + \sigma_{yx}y_2 + \sigma_{zx}z_2)] e_{ikl} w_i w_k,$$

along face four, where $dA = -(x_2 e_x + y_2 e_y + z_2 e_z) drdt$; (B.4.8)

$$M_x^{5e} = -\sum_{jk} [\chi_y(\sigma_{xz}x_1 + \sigma_{yz}y_1 + \sigma_{zz}z_1) - \chi_z(\sigma_{xy}x_1 + \sigma_{yy}y_1 + \sigma_{zy}z_1)] e_{ijk} w_j w_k,$$

$$M_y^{5e} = -\sum_{jk} [\chi_z(\sigma_{xx}x_1 + \sigma_{yx}y_1 + \sigma_{zx}z_1) - \chi_x(\sigma_{xz}x_1 + \sigma_{yz}y_1 + \sigma_{zz}z_1)] e_{ijk} w_j w_k,$$

$$M_z^{5e} = -\sum_{jk} [\chi_x(\sigma_{xy}x_1 + \sigma_{yy}y_1 + \sigma_{zy}z_1) - \chi_y(\sigma_{xx}x_1 + \sigma_{yx}y_1 + \sigma_{zx}z_1)] e_{ijk} w_j w_k,$$

along face five, where $dA = -(x_1 e_x + y_1 e_y + z_1 e_z) dsdt$; (B.4.9)

$$M_x^{6e} = \sum_{jk} [\chi_y(\sigma_{xz}x_1 + \sigma_{yz}y_1 + \sigma_{zz}z_1) - \chi_z(\sigma_{xy}x_1 + \sigma_{yy}y_1 + \sigma_{zy}z_1)] e_{itjk} w_j w_k,$$

$$M_y^{6e} = \sum_{jk} [\chi_z(\sigma_{xx}x_1 + \sigma_{yx}y_1 + \sigma_{zx}z_1) - \chi_x(\sigma_{xz}x_1 + \sigma_{yz}y_1 + \sigma_{zz}z_1)] e_{itjk} w_j w_k,$$

$$M_z^{6e} = \sum_{jk} [\chi_x(\sigma_{xy}x_1 + \sigma_{yy}y_1 + \sigma_{zy}z_1) - \chi_y(\sigma_{xx}x_1 + \sigma_{yx}y_1 + \sigma_{zx}z_1)] e_{itjk} w_j w_k,$$

along face six, where $dA = (x_1 e_x + y_1 e_y + z_1 e_z) dsdt$. (B.4.10)

APPENDIX C

IMPERMEABLE WALL BOUNDARY CONDITIONS

C.1 Physical Basis

Along an impermeable wall the normal fluid velocity must equal the normal component of the wall velocity, while the tangential velocity may vary. We express this as

$$\mathbf{n} \cdot \mathbf{V} = \mathbf{n} \cdot \mathbf{V}_{\text{wall}}. \quad (\text{C.1.1})$$

Another condition on impermeable wall boundaries requires zero tangential stress, or, equivalently, that the stress points normal to the surface. In other words, the cross product of the surface unit normal and the local stress vector equals zero. Thus, an impermeable wall, unlike a solid wall, cannot support a tangential stress. In symbolic form this boundary condition equals

$$\mathbf{n} \times (\underline{\sigma} \cdot \mathbf{n}) = 0, \quad (\text{C.1.2})$$

where \mathbf{n} represents the surface outward unit normal vector, and $\underline{\sigma}$ represents the total stress tensor consisting of the sum of the isotropic and deviatoric terms. We must prove that the combination of these two boundary conditions equals the single condition given by

$$(\mathbf{n} \cdot \nabla) \mathbf{V} = 0. \quad (\text{C.2.1})$$

The derivation of this relation follows.

C.2 Mathematical Derivation

Begin by expressing the unit normal as

$$\mathbf{n} = n_x \mathbf{e}_x + n_y \mathbf{e}_y + n_z \mathbf{e}_z \quad (\text{C.2.2})$$

and the velocity as

$$\mathbf{V} = U \mathbf{e}_x + V \mathbf{e}_y + W \mathbf{e}_z. \quad (\text{C.2.3})$$

The inner product $\mathbf{n} \cdot \mathbf{V}$ gives

$$\mathbf{n} \cdot \mathbf{V} = U n_x + V n_y + W n_z. \quad (\text{C.2.4})$$

Setting this equal to the normal velocity of the boundary gives

$$U n_x + V n_y + W n_z = \mathbf{n} \cdot \mathbf{V}_{\text{wall}}. \quad (\text{C.2.5})$$

The stress vector on a surface with normal, \mathbf{n} , equals $\mathbf{t}(\mathbf{n})$ which appears as

$$\mathbf{t}(\mathbf{n}) = \underline{\sigma} \cdot \mathbf{n} = \quad (\text{C.2.6})$$

$$\begin{aligned} & (\sigma_{xx} n_x + \sigma_{yx} n_y + \sigma_{zx} n_z) \mathbf{e}_x + \\ & (\sigma_{xy} n_x + \sigma_{yy} n_y + \sigma_{zy} n_z) \mathbf{e}_y + \\ & (\sigma_{xz} n_x + \sigma_{yz} n_y + \sigma_{zz} n_z) \mathbf{e}_z \end{aligned}$$

according to appendix B. The cross product of this relation with the unit normal equals

$$\mathbf{n} \times \mathbf{t}(\mathbf{n}) = \mathbf{n} \times \underline{\sigma} \cdot \mathbf{n} = \quad (\text{C.2.7})$$

$$\begin{aligned} & [n_y(\sigma_{xz} n_x + \sigma_{yz} n_y + \sigma_{zz} n_z) - n_z(\sigma_{xy} n_x + \sigma_{yy} n_y + \sigma_{zy} n_z)] \mathbf{e}_x + \\ & [n_z(\sigma_{xx} n_x + \sigma_{yx} n_y + \sigma_{zx} n_z) - n_x(\sigma_{xz} n_x + \sigma_{yz} n_y + \sigma_{zz} n_z)] \mathbf{e}_y + \\ & [n_x(\sigma_{xy} n_x + \sigma_{yy} n_y + \sigma_{zy} n_z) - n_y(\sigma_{xx} n_x + \sigma_{yx} n_y + \sigma_{zx} n_z)] \mathbf{e}_z. \end{aligned}$$

Using (B.2.1) through (B.2.4) for the stress components gives the following relations for the three components of the above expression:

$$\begin{aligned} (\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_x &= \mu n_x n_y \left(\frac{\partial U}{\partial z} + \frac{\partial W}{\partial x} \right) + \mu n_y n_y \left(\frac{\partial W}{\partial y} + \frac{\partial V}{\partial z} \right) + \mu n_z n_y (2 \frac{\partial W}{\partial z} - p) - \\ & \mu n_x n_z \left(\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right) - \mu n_y n_z (2 \frac{\partial V}{\partial y} - p) - \mu n_z n_z \left(\frac{\partial V}{\partial z} + \frac{\partial W}{\partial y} \right), \quad (\text{C.2.8}) \end{aligned}$$

$$\begin{aligned} (\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_y &= \mu n_x n_z (2 \frac{\partial U}{\partial x} - p) + \mu n_y n_z \left(\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right) + \mu n_z n_z \left(\frac{\partial W}{\partial x} + \frac{\partial U}{\partial z} \right) - \\ & \mu n_x n_x \left(\frac{\partial U}{\partial z} + \frac{\partial W}{\partial x} \right) - \mu n_y n_x \left(\frac{\partial W}{\partial y} + \frac{\partial V}{\partial z} \right) - \mu n_z n_x (2 \frac{\partial W}{\partial z} - p), \quad (\text{C.2.9}) \end{aligned}$$

$$\begin{aligned} (\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_z &= \mu n_x n_x \left(\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right) + \mu n_y n_x (2 \frac{\partial V}{\partial y} - p) + \mu n_z n_x \left(\frac{\partial W}{\partial y} + \frac{\partial V}{\partial z} \right) - \\ & \mu n_x n_y (2 \frac{\partial U}{\partial x} - p) - \mu n_y n_y \left(\frac{\partial V}{\partial x} + \frac{\partial U}{\partial y} \right) - \mu n_z n_y \left(\frac{\partial V}{\partial z} + \frac{\partial W}{\partial y} \right). \quad (\text{C.2.10}) \end{aligned}$$

The pressure terms cancel in each of these expressions giving

$$\begin{aligned} (\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_x &= \mu n_x n_y \left(\frac{\partial U}{\partial z} + \frac{\partial W}{\partial x} \right) + \mu n_y n_y \left(\frac{\partial W}{\partial y} + \frac{\partial V}{\partial z} \right) + \mu n_z n_y (2 \frac{\partial W}{\partial z} - 2 \frac{\partial V}{\partial y}) - \\ & \mu n_x n_z \left(\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right) - \mu n_z n_z \left(\frac{\partial V}{\partial z} + \frac{\partial W}{\partial y} \right), \quad (\text{C.2.11}) \end{aligned}$$

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_y = \mu n_x n_z (2 \frac{\partial U}{\partial x} - 2 \frac{\partial W}{\partial z}) + \mu n_y n_z (\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x}) + \mu n_z n_x (\frac{\partial W}{\partial x} + \frac{\partial U}{\partial z}) - \mu n_x n_x (\frac{\partial U}{\partial z} + \frac{\partial W}{\partial x}) - \mu n_y n_x (\frac{\partial W}{\partial y} + \frac{\partial V}{\partial z}), \quad (\text{C.2.12})$$

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_z = \mu n_x n_x (\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x}) + \mu n_y n_x (2 \frac{\partial V}{\partial y} - 2 \frac{\partial U}{\partial x}) + \mu n_z n_x (\frac{\partial W}{\partial y} + \frac{\partial V}{\partial z}) - \mu n_y n_y (\frac{\partial V}{\partial x} + \frac{\partial U}{\partial y}) - \mu n_z n_y (\frac{\partial V}{\partial z} + \frac{\partial W}{\partial y}). \quad (\text{C.2.13})$$

After further rearrangement we obtain

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_x = -\mu n_z (n_x \frac{\partial U}{\partial y} + n_y \frac{\partial V}{\partial y} + n_z \frac{\partial W}{\partial y}) + \mu n_y (n_x \frac{\partial U}{\partial z} + n_y \frac{\partial V}{\partial z} + n_z \frac{\partial W}{\partial z}) + \mu (n_x \frac{\partial}{\partial x} + n_y \frac{\partial}{\partial y} + n_z \frac{\partial}{\partial z}) (n_y W - n_z V), \quad (\text{C.2.14})$$

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_y = -\mu n_x (n_x \frac{\partial U}{\partial z} + n_y \frac{\partial V}{\partial z} + n_z \frac{\partial W}{\partial z}) + \mu n_z (n_x \frac{\partial U}{\partial x} + n_y \frac{\partial V}{\partial x} + n_z \frac{\partial W}{\partial x}) + \mu (n_x \frac{\partial}{\partial x} + n_y \frac{\partial}{\partial y} + n_z \frac{\partial}{\partial z}) (n_z U - n_x W), \quad (\text{C.2.15})$$

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_z = -\mu n_y (n_x \frac{\partial U}{\partial x} + n_y \frac{\partial V}{\partial x} + n_z \frac{\partial W}{\partial x}) + \mu n_x (n_x \frac{\partial U}{\partial y} + n_y \frac{\partial V}{\partial y} + n_z \frac{\partial W}{\partial y}) + \mu (n_x \frac{\partial}{\partial x} + n_y \frac{\partial}{\partial y} + n_z \frac{\partial}{\partial z}) (n_x V - n_y U). \quad (\text{C.2.16})$$

The partial derivatives of the unit normal vector with respect to the spatial co-ordinates differ from zero on a curved surface. Hence, we cannot interchange the derivative operator in the first two terms of each expression with the components of the normal vector (e.g., $n_x \frac{\partial U}{\partial y} + n_y \frac{\partial V}{\partial y} + n_z \frac{\partial W}{\partial y} \neq \frac{\partial}{\partial y} (n_x U + n_y V + n_z W)$).

However, the derivative may move outside the components of the normal vector if we only consider surfaces with zero curvature. When we restrict ourselves to this case, the above relations may appear as

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_x = -\mu n_z \frac{\partial}{\partial y} (n_x U + n_y V + n_z W) + \mu n_y \frac{\partial}{\partial z} (n_x U + n_y V + n_z W) + \mu (n_x \frac{\partial}{\partial x} + n_y \frac{\partial}{\partial y} + n_z \frac{\partial}{\partial z}) (n_y W - n_z V), \quad (\text{C.2.17})$$

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_y = -\mu n_x \frac{\partial}{\partial z} (n_x U + n_y V + n_z W) + \mu n_z \frac{\partial}{\partial x} (n_x U + n_y V + n_z W) + \mu (n_x \frac{\partial}{\partial x} + n_y \frac{\partial}{\partial y} + n_z \frac{\partial}{\partial z}) (n_z U - n_x W), \quad (\text{C.2.18})$$

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_z = -\mu n_y \frac{\partial}{\partial x} (n_x U + n_y V + n_z W) + \mu n_x \frac{\partial}{\partial y} (n_x U + n_y V + n_z W) + \mu (n_x \frac{\partial}{\partial x} + n_y \frac{\partial}{\partial y} + n_z \frac{\partial}{\partial z}) (n_x V - n_y U). \quad (\text{C.2.19})$$

Introducing $\mathbf{n} \cdot \mathbf{V} = n_x U + n_y V + n_z W$ and $\mathbf{n} \cdot \nabla = n_x \frac{\partial}{\partial x} + n_y \frac{\partial}{\partial y} + n_z \frac{\partial}{\partial z}$ into these

expressions yields

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_x = \mu \left(n_y \frac{\partial}{\partial z} - n_z \frac{\partial}{\partial y} \right) \mathbf{n} \cdot \mathbf{V} + \mu \mathbf{n} \cdot \nabla (n_y W - n_z V), \quad (\text{C.2.20})$$

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_y = -\mu \left(n_x \frac{\partial}{\partial z} - n_z \frac{\partial}{\partial x} \right) \mathbf{n} \cdot \mathbf{V} + \mu \mathbf{n} \cdot \nabla (n_z U - n_x W), \quad (\text{C.2.21})$$

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})_z = -\mu \left(n_y \frac{\partial}{\partial x} - n_x \frac{\partial}{\partial y} \right) \mathbf{n} \cdot \mathbf{V} + \mu \mathbf{n} \cdot \nabla (n_x V - n_y U). \quad (\text{C.2.22})$$

After introducing the cross product, the three components of $(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n})$ reduce to a single vector expression given by

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n}) = \mu [(\mathbf{n} \times \nabla) \mathbf{n} \cdot \mathbf{V} + (\mathbf{n} \cdot \nabla) \mathbf{n} \times \mathbf{V}]. \quad (\text{C.2.23})$$

This equation also appears as

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n}) = \mu \mathbf{n} \times [\nabla (\mathbf{n} \cdot \mathbf{V}) + (\mathbf{n} \cdot \nabla) \mathbf{V}]. \quad (\text{C.2.24})$$

Introducing $\mathbf{n} \cdot \mathbf{V} = \mathbf{n} \cdot \mathbf{V}_{\text{wall}}$ gives

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n}) = \mu \mathbf{n} \times [\nabla (\mathbf{n} \cdot \mathbf{V}_{\text{wall}}) + (\mathbf{n} \cdot \nabla) \mathbf{V}]. \quad (\text{C.2.25})$$

For a general curved boundary moving with velocity \mathbf{V}_{wall} , the quantity $\nabla (\mathbf{n} \cdot \mathbf{V}_{\text{wall}})$, does not equal zero. However, since we are limiting our consideration to flat boundaries, this term does equal zero. In this case the boundary condition reduces to

$$(\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n}) = \mu \mathbf{n} \times [(\mathbf{n} \cdot \nabla) \mathbf{V}]. \quad (\text{C.2.26})$$

Since the original boundary condition, $\mathbf{n} \times \underline{\sigma} \cdot \mathbf{n}$, equals zero, we require

$$\mu \mathbf{n} \times [(\mathbf{n} \cdot \nabla) \mathbf{V}] = \mu (\mathbf{n} \cdot \nabla) (\mathbf{n} \times \mathbf{V}) = 0. \quad (\text{C.2.27})$$

This equation is satisfied when the unit normal lies parallel to the velocity vector giving $\mathbf{n} \times \mathbf{V} = 0$. This seems like a most unusual condition and we assume that it does not hold for most boundaries. The other possibility requires

$$(\mathbf{n} \cdot \nabla) \mathbf{V} = 0, \quad (\text{C.2.28})$$

and represents the desired form of the boundary conditions given in §C.1. This proves that the two impermeable wall boundary conditions reduce to homogeneous natural conditions when we enforce (1) zero surface curvature to

ensure $\nabla(\mathbf{n} \cdot \mathbf{V}_{\text{wall}}) = 0$, and (2) a surface with unit normal not parallel to the local velocity.

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